

## Supplementary Information

# Unravelling the kinetics of electro- and photochemical S→O linkage isomerization in Ru(II)-NHC-DMSO complexes utilised for photoinduced substitution reactions

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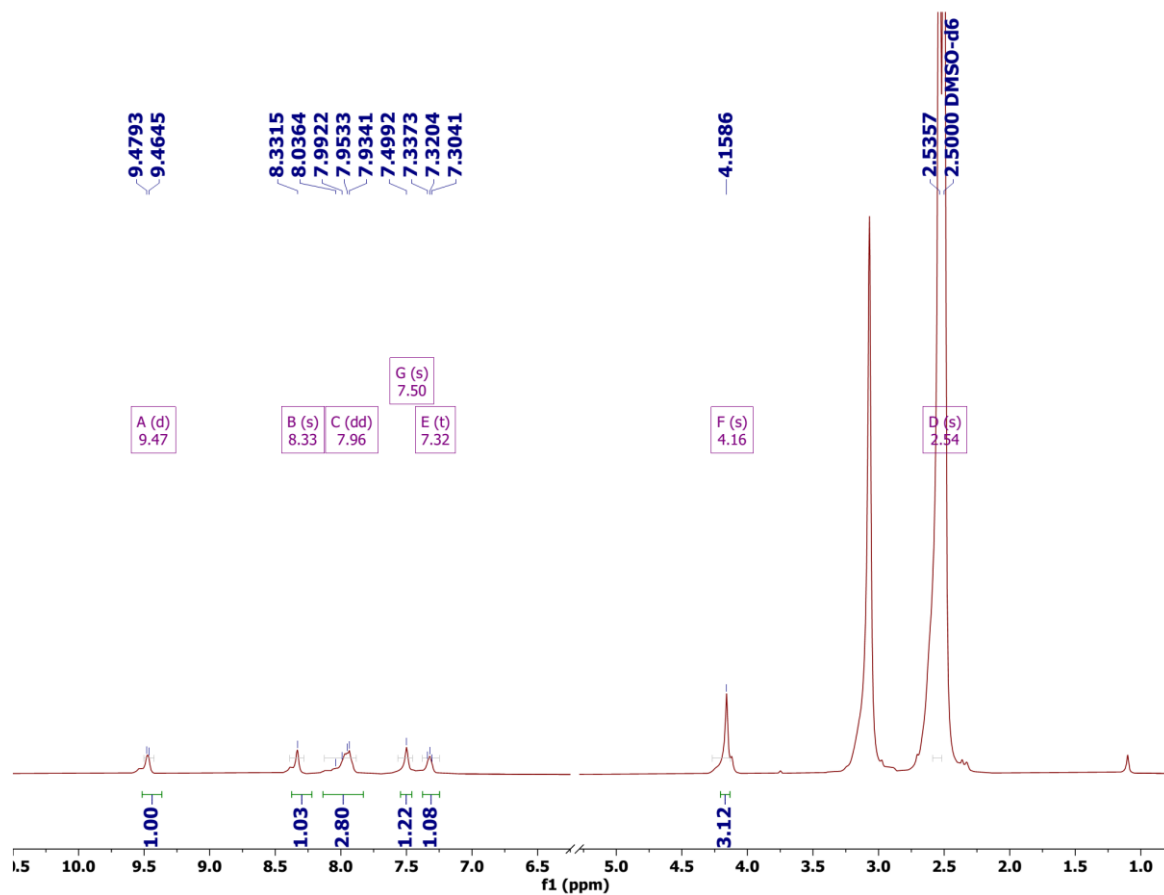
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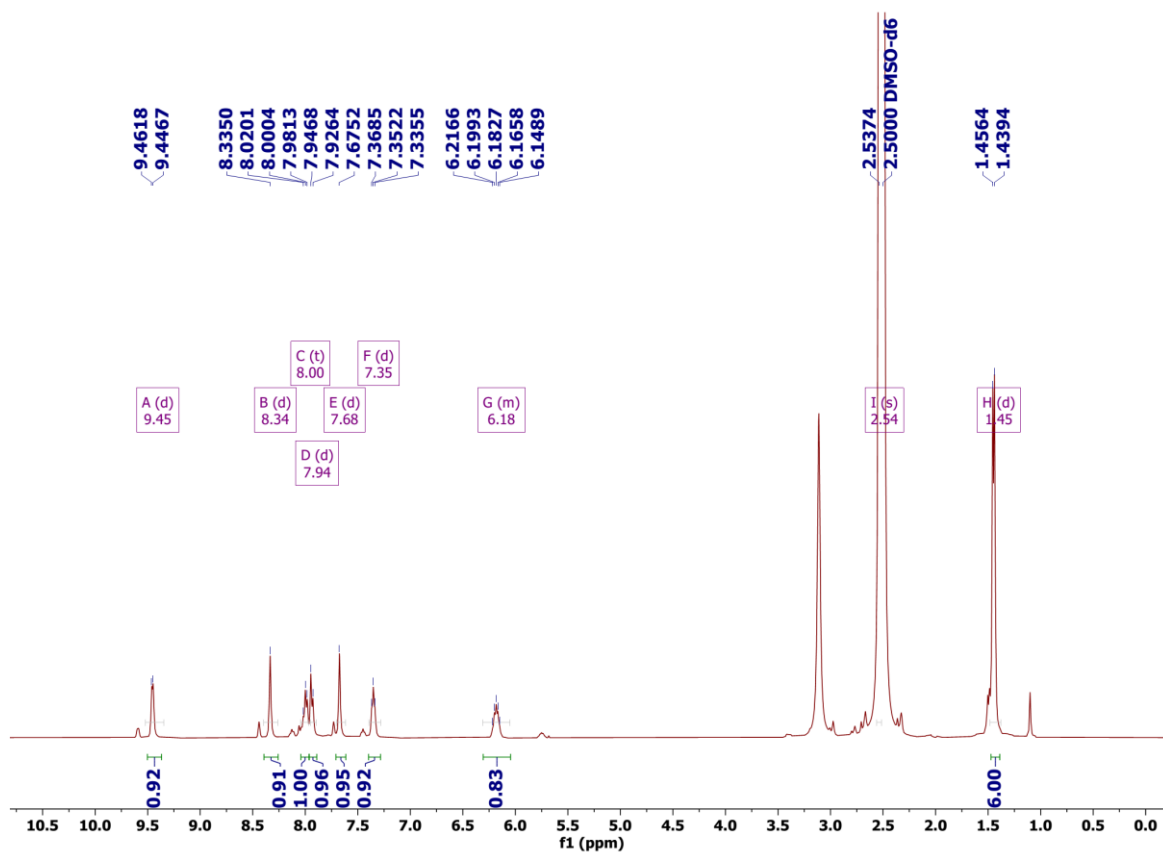
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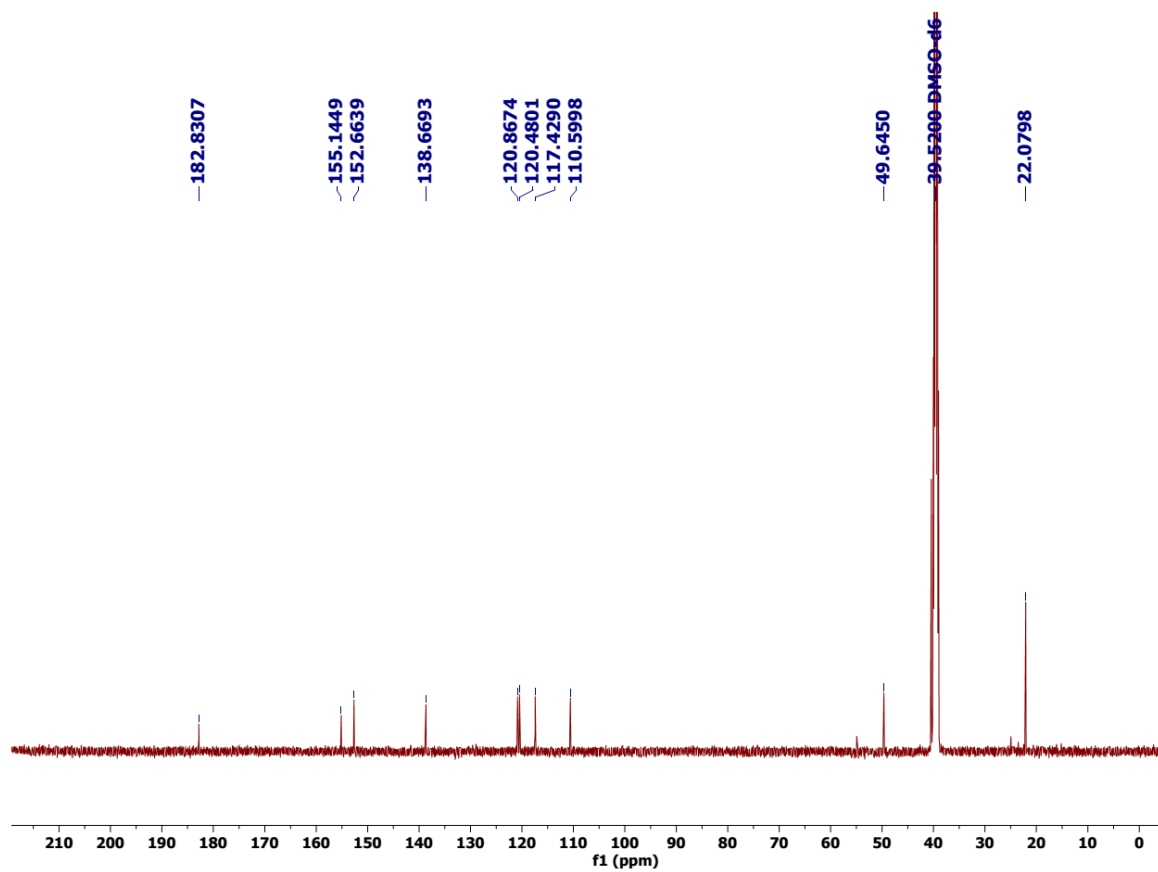
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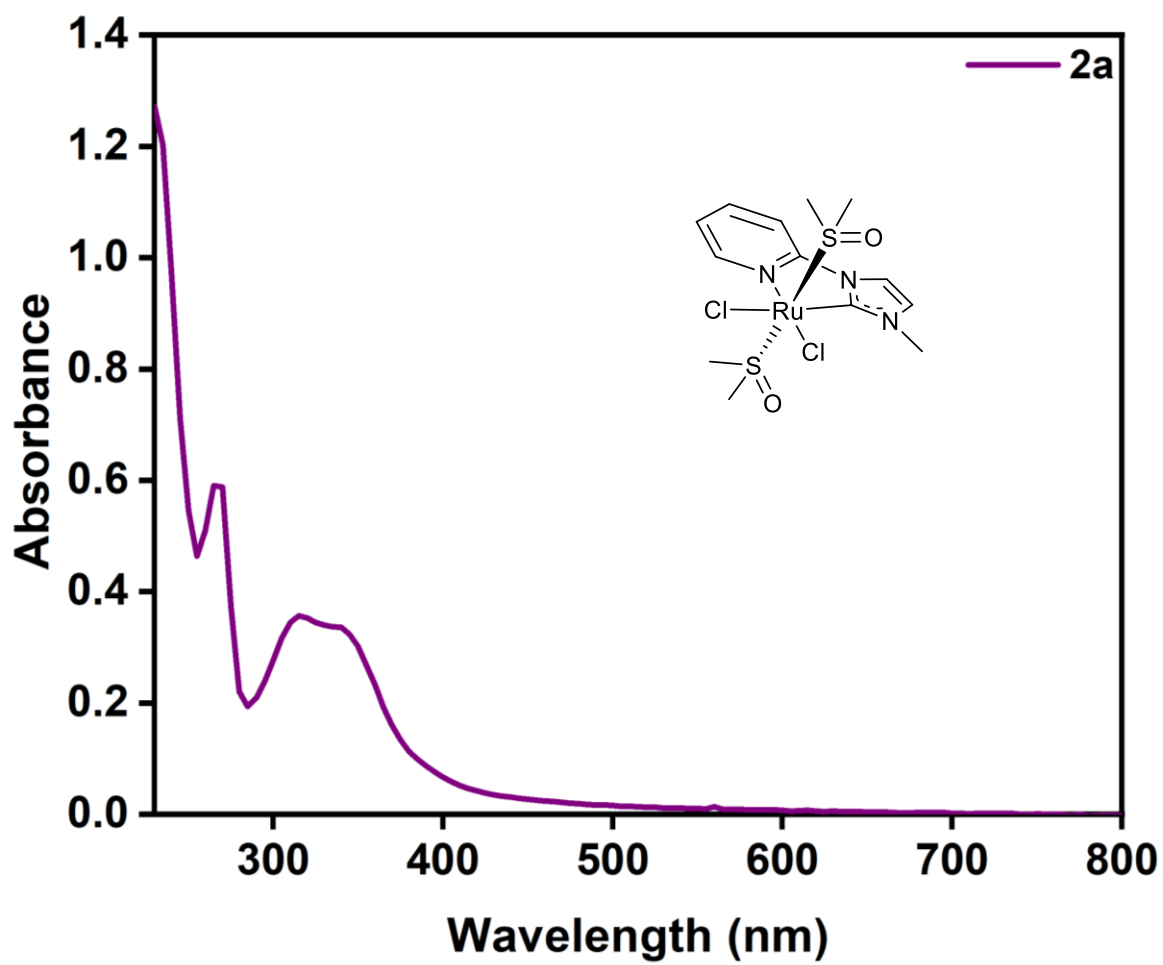
**Figure S1.**  $^1\text{H}$  NMR of complex **2a** recorded in  $\text{DMSO-d}_6$  at temperature 350 K.



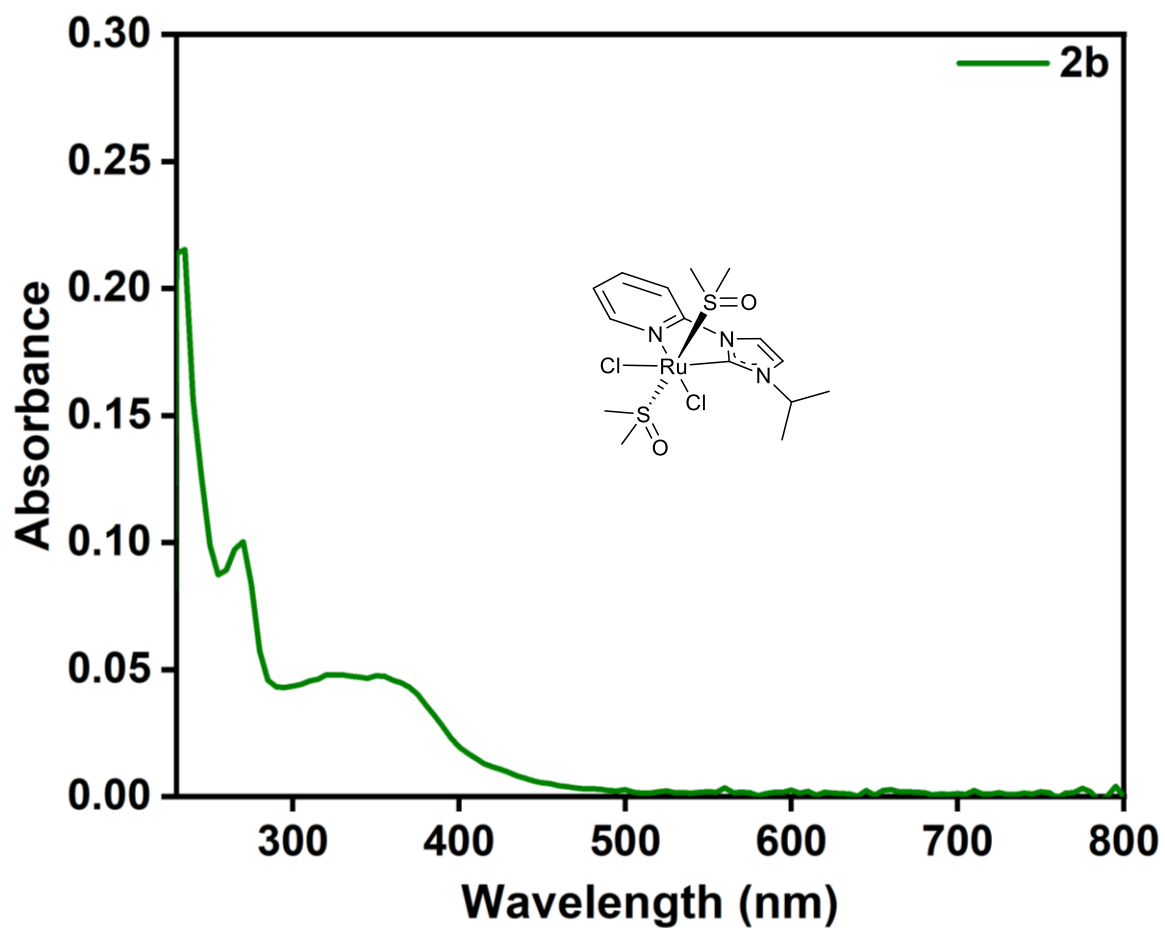
**Figure S2.**  $^1\text{H}$  NMR spectrum of complex **2b** recorded in DMSO- $\text{d}_6$  at temperature 350 K.



**Figure S3.**  $^{13}\text{C}$  NMR of complex **2b** recorded in  $\text{DMSO-d}_6$  at temperature 350 K.



**Figure S4.** UV-Vis spectrum of complex **2a** recorded in MeOH at room temperature.



**Figure S5.** UV-Vis spectrum of complex **2b** recorded in MeOH at room temperature.



## Generic Display Report

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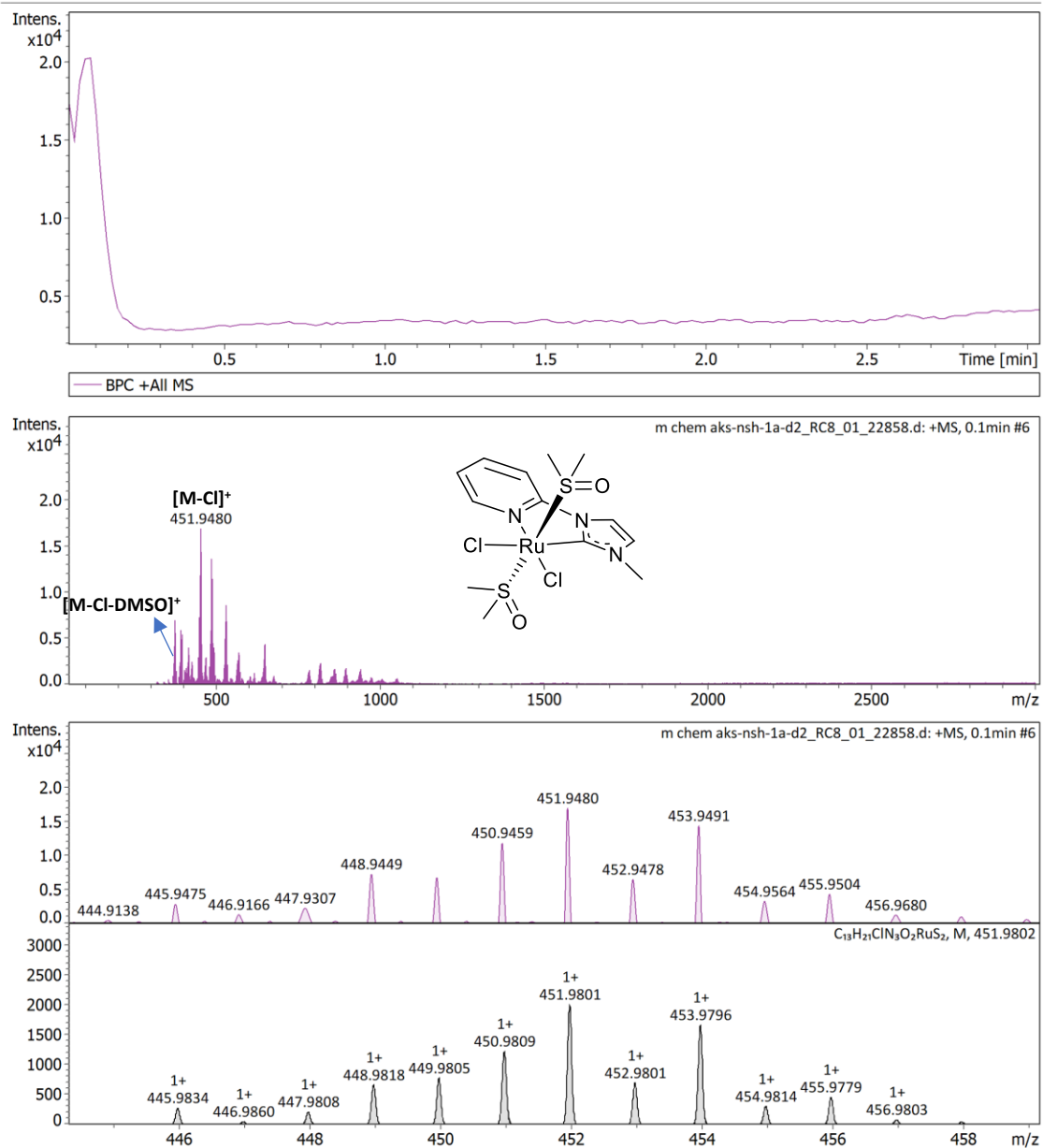
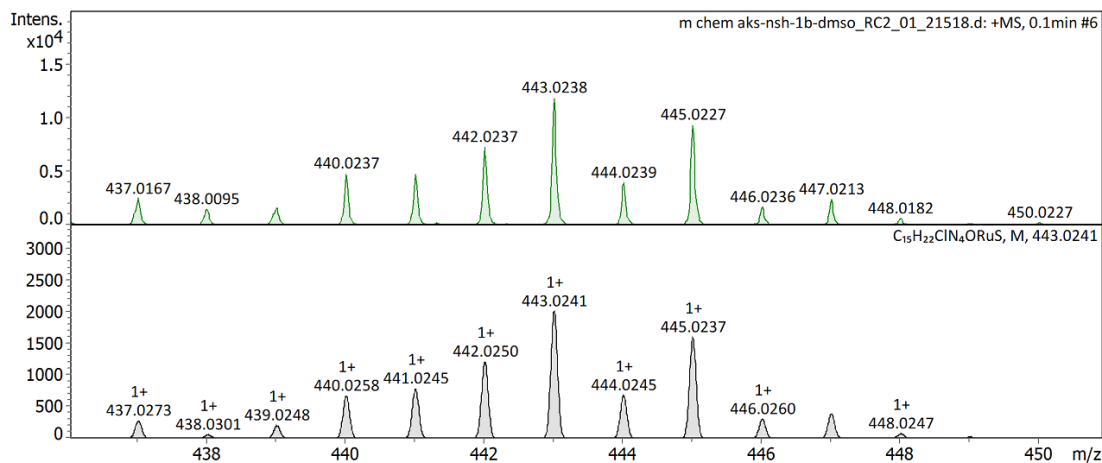
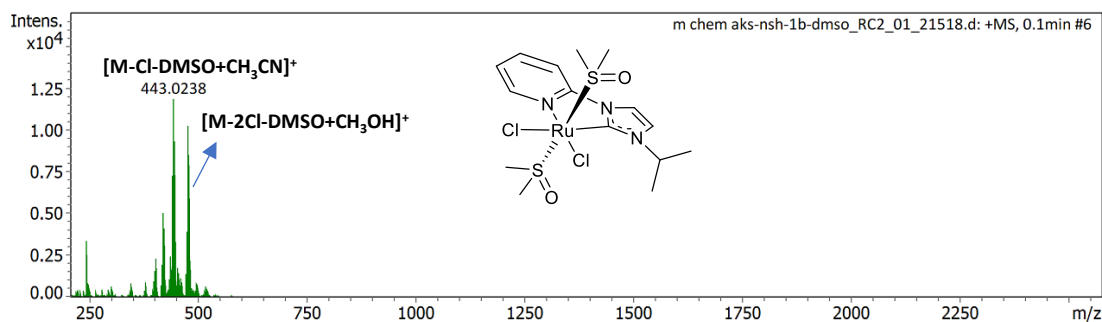
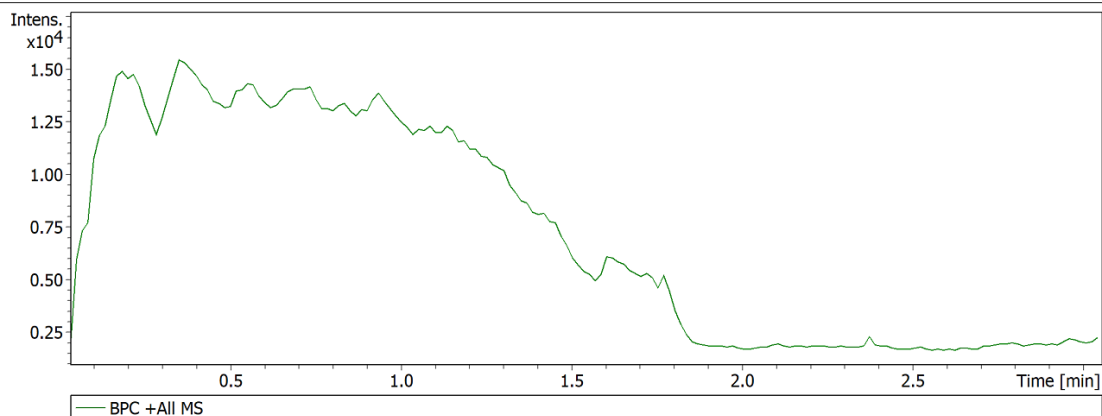


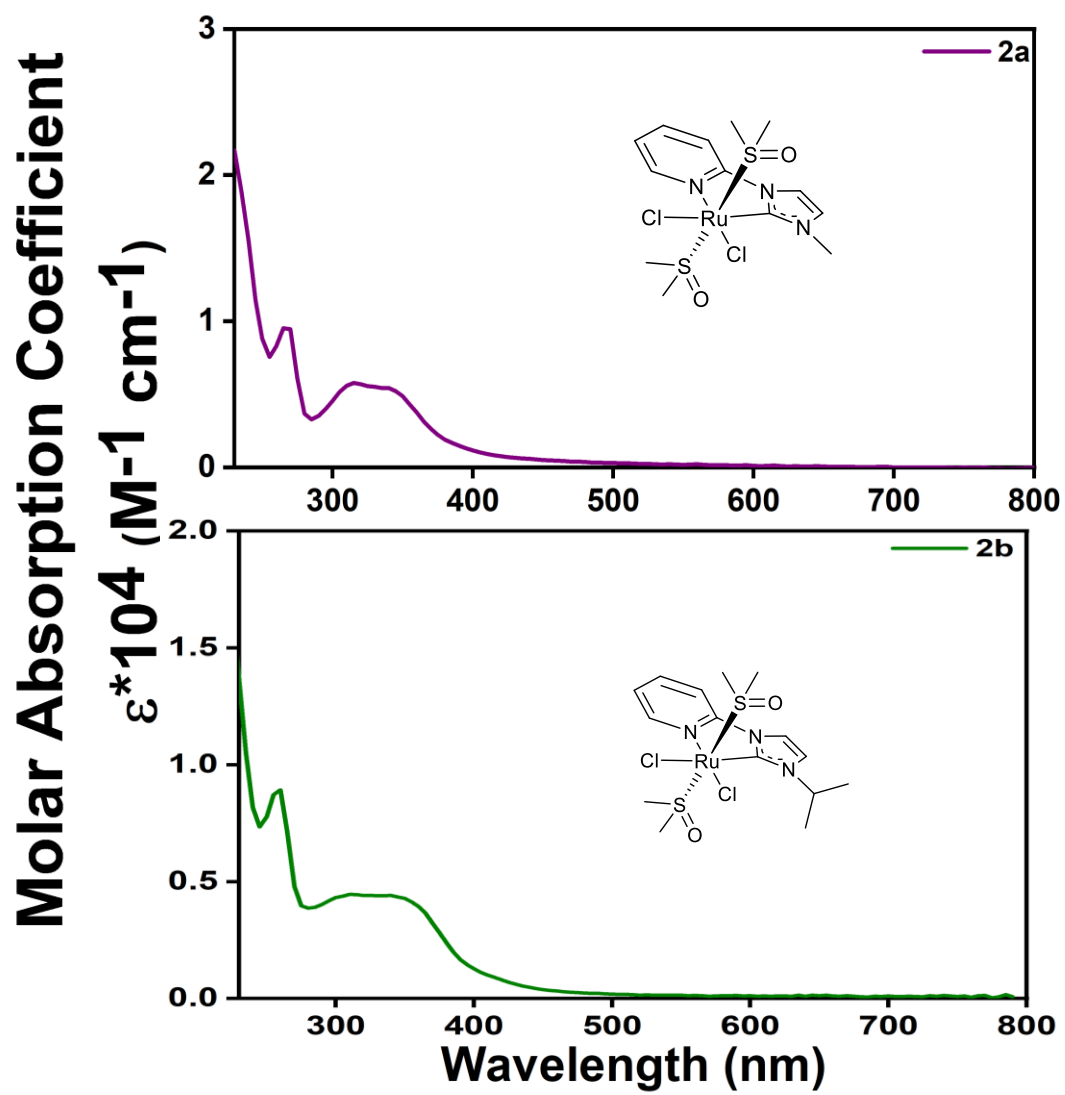
Figure S6. LCMS of complex 2a.

## Generic Display Report

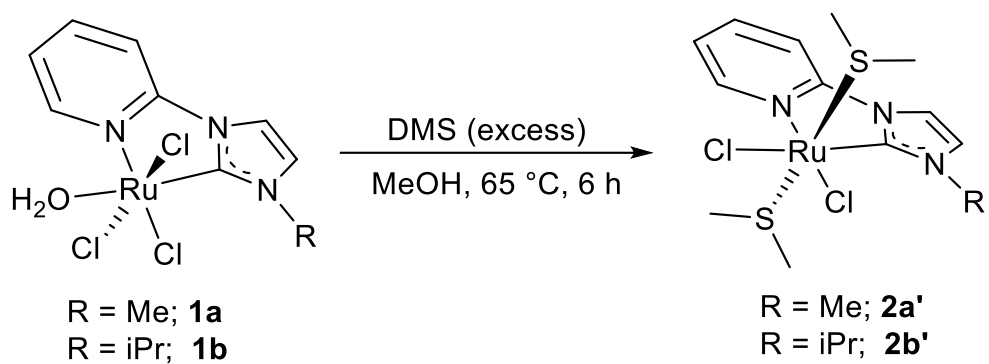
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Comment			



**Figure S7.** LCMS and HRMS of complex **2b**.



**Figure S8.** Stack plots of Molar absorption coefficients of complexes **2a** (up) and **2b** (down) recorded in DCM at room temperature.



**Scheme S1.** Synthesis of Ru(II)-PyNHC-(DMS)<sub>2</sub> complexes **2a'** and **2b'** from Ru(III)-NHC complexes **1a** and **1b** respectively.

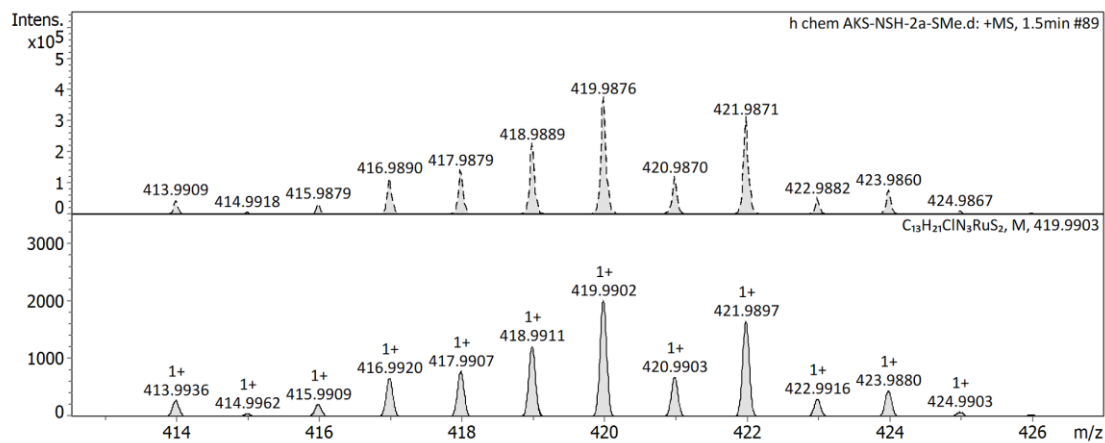
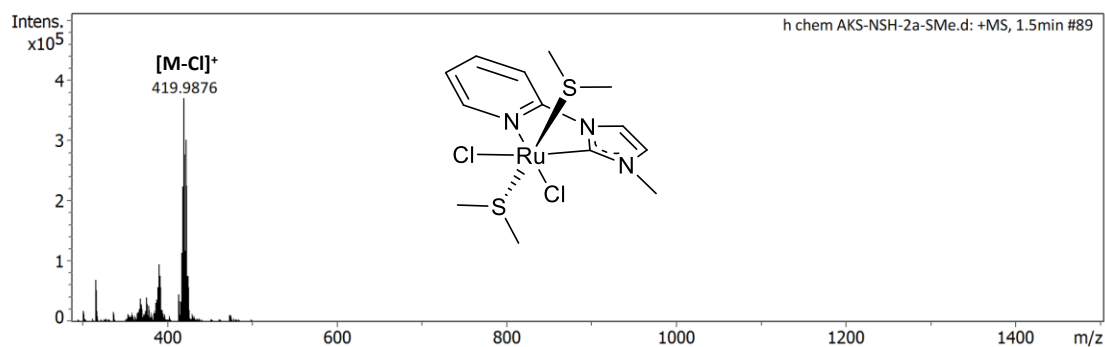
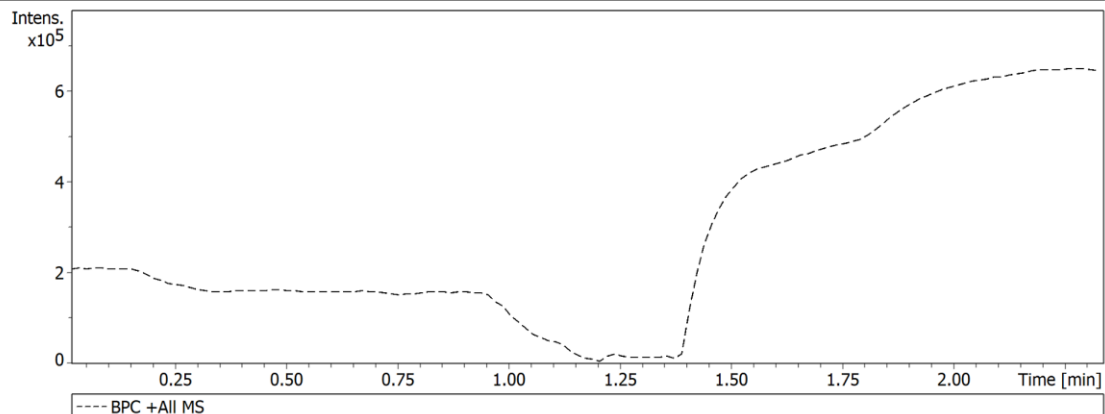
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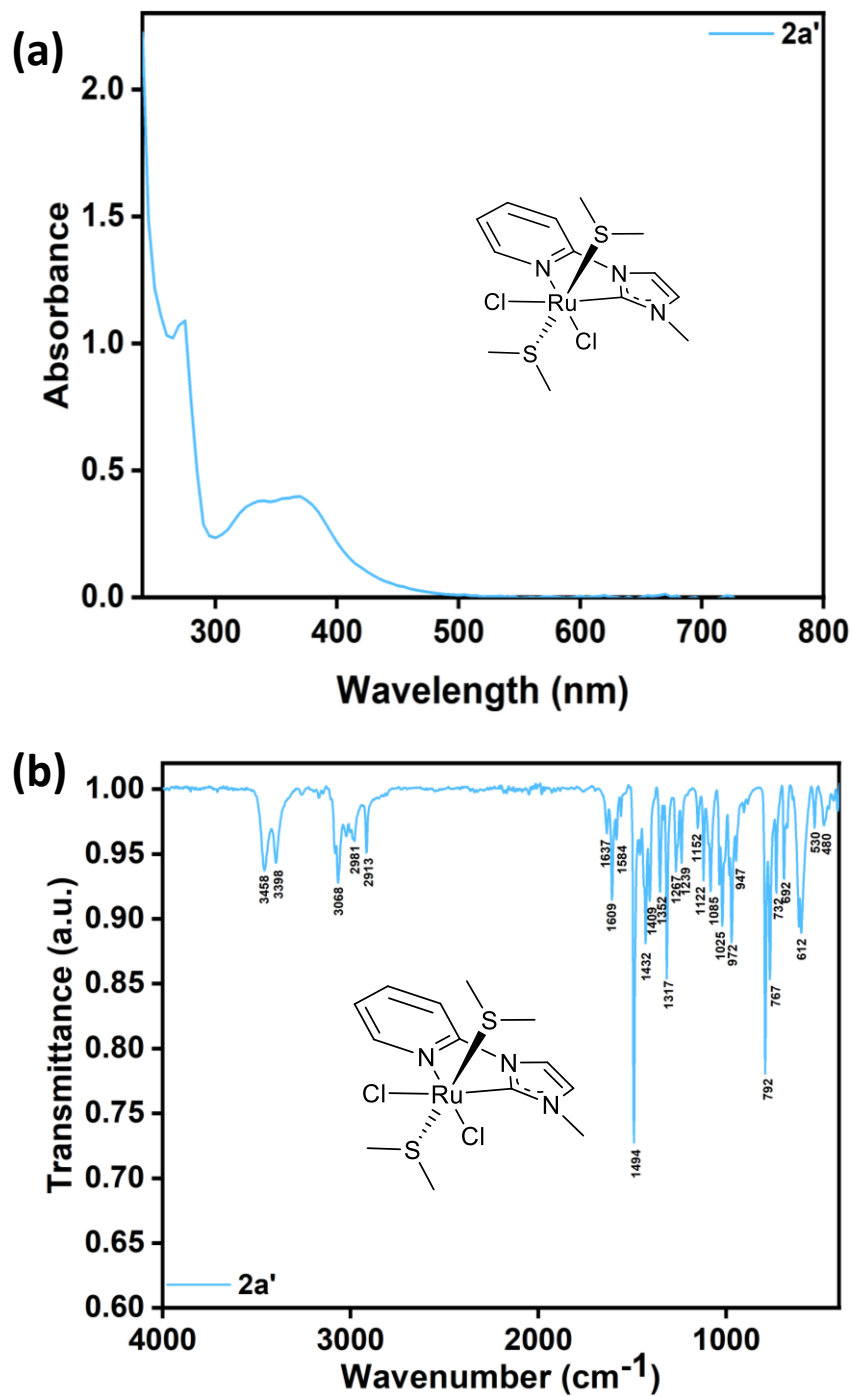
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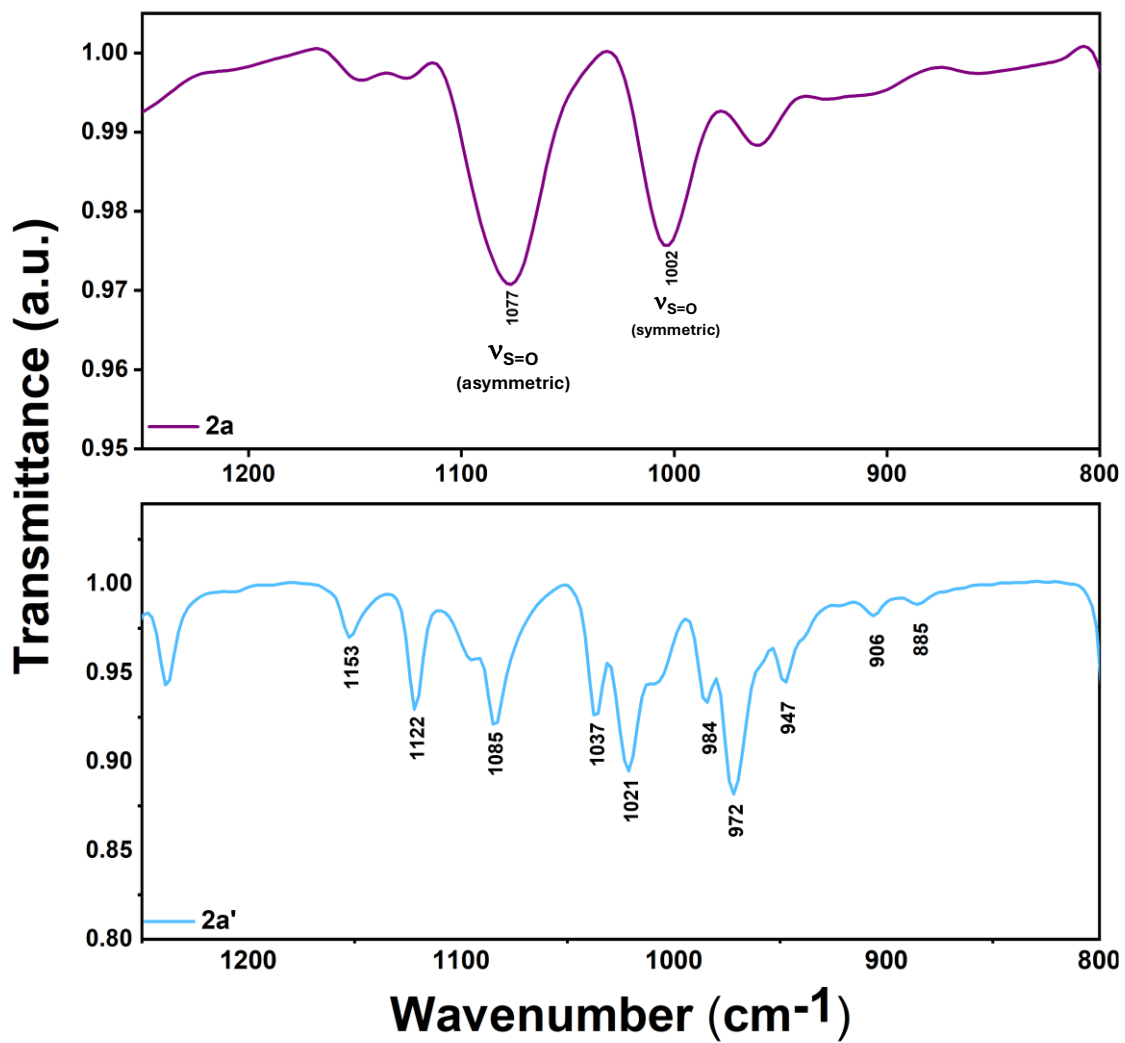
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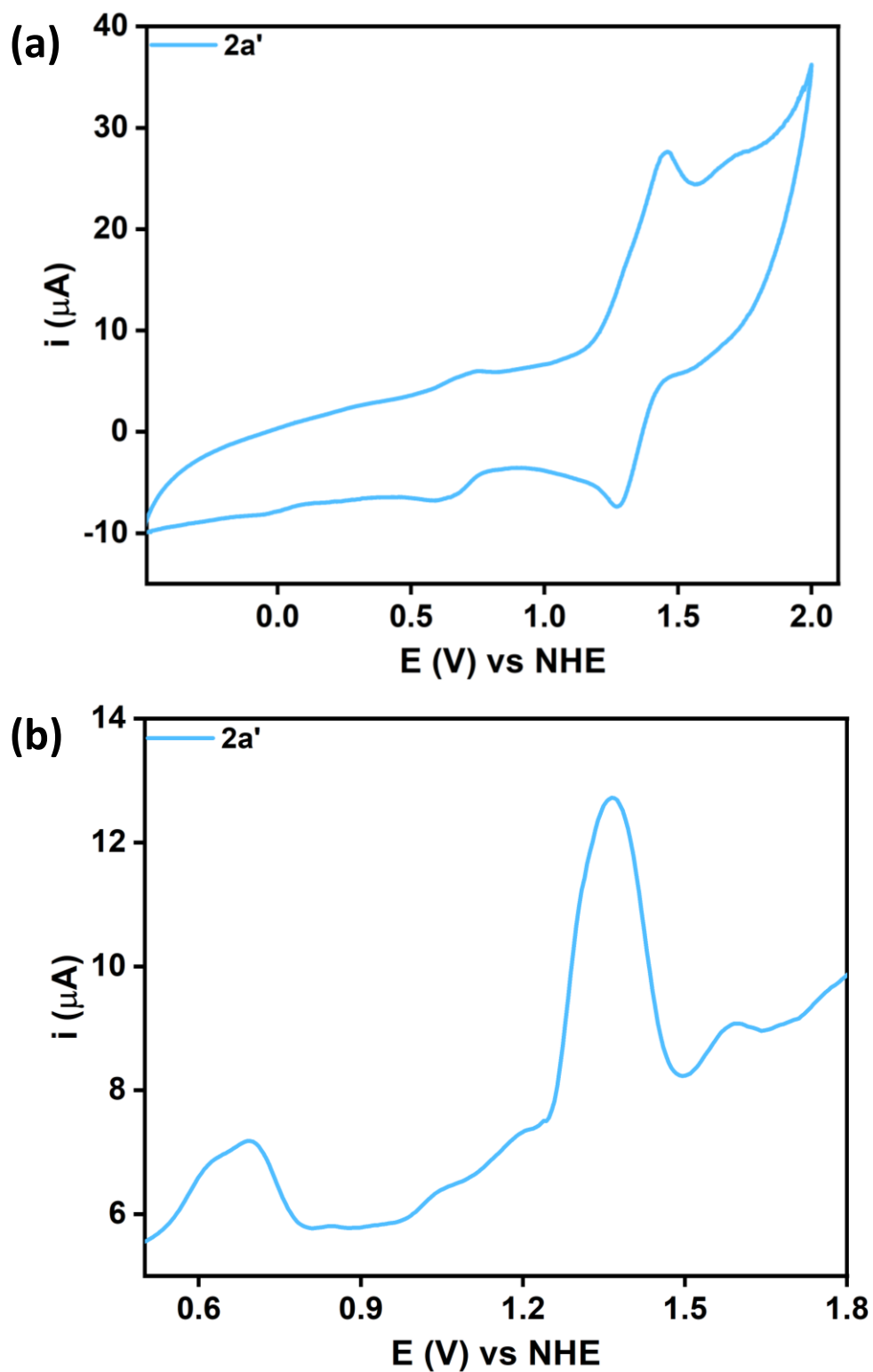
**Figure S9.** LCMS and HRMS of complex **2a'**.



**Figure S10.** (a) UV-Vis spectrum of complex **2a'** recorded in MeOH at room temperature and (b) FT-IR spectrum of complex **2a'** recorded in solid state.



**Figure S11.** Comparative IR spectra of **2a** (up) and **2a'** (down) for the identification of IR bands for S=O in Ru-NHC-(DMSO)<sub>2</sub> complex.



**Figure S12.** (a) Cyclic voltammogram and (b) DPV of complex **2a'** recorded in  $\text{CH}_2\text{Cl}_2$  using 0.1 M  $\text{NH}_4\text{PF}_6$  as the supporting electrolyte.



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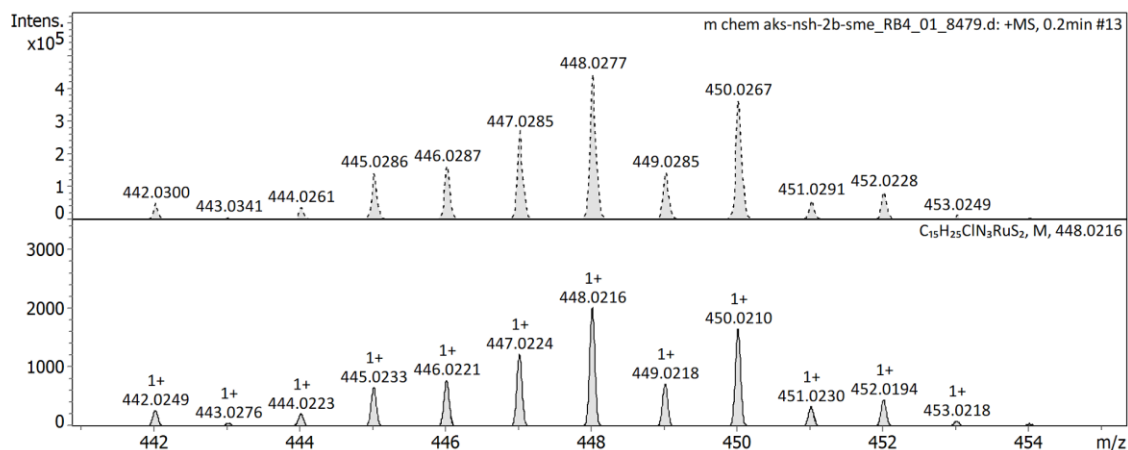
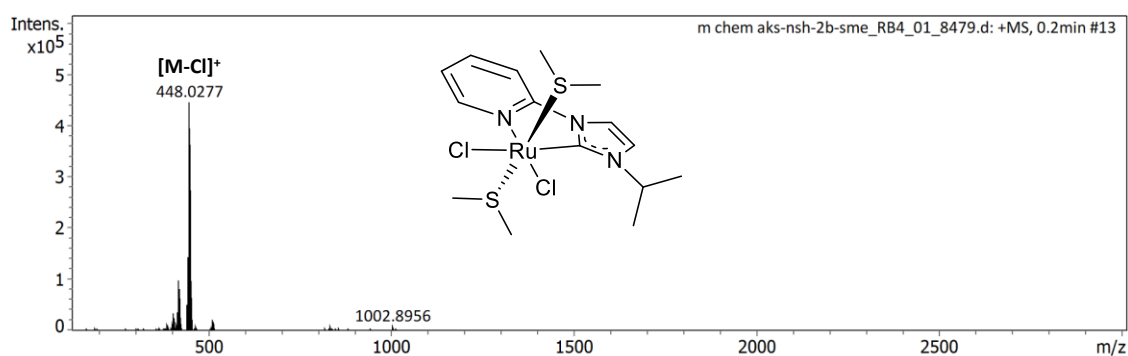
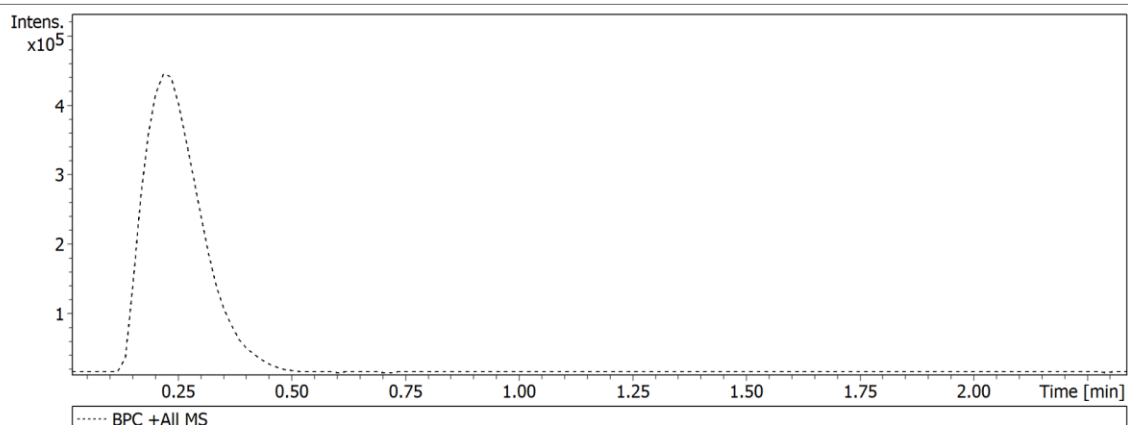
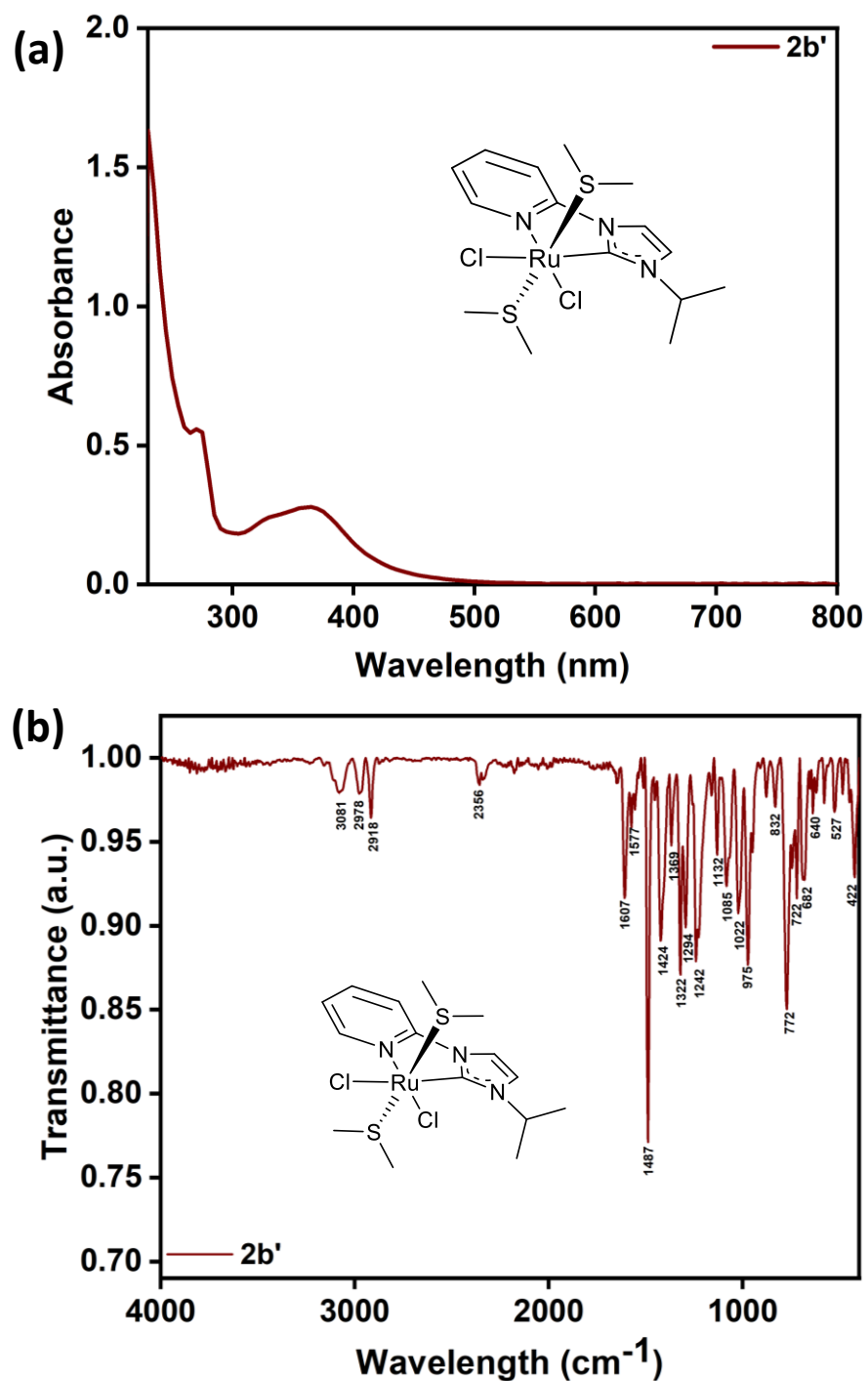


Figure S13. LCMS and HRMS of complex **2b'**.



**Figure S14.** (a) UV-Vis spectrum of complex **2b'** recorded in MeOH at room temperature and (b) FT-IR spectrum of complex **2b'** recorded in solid state.

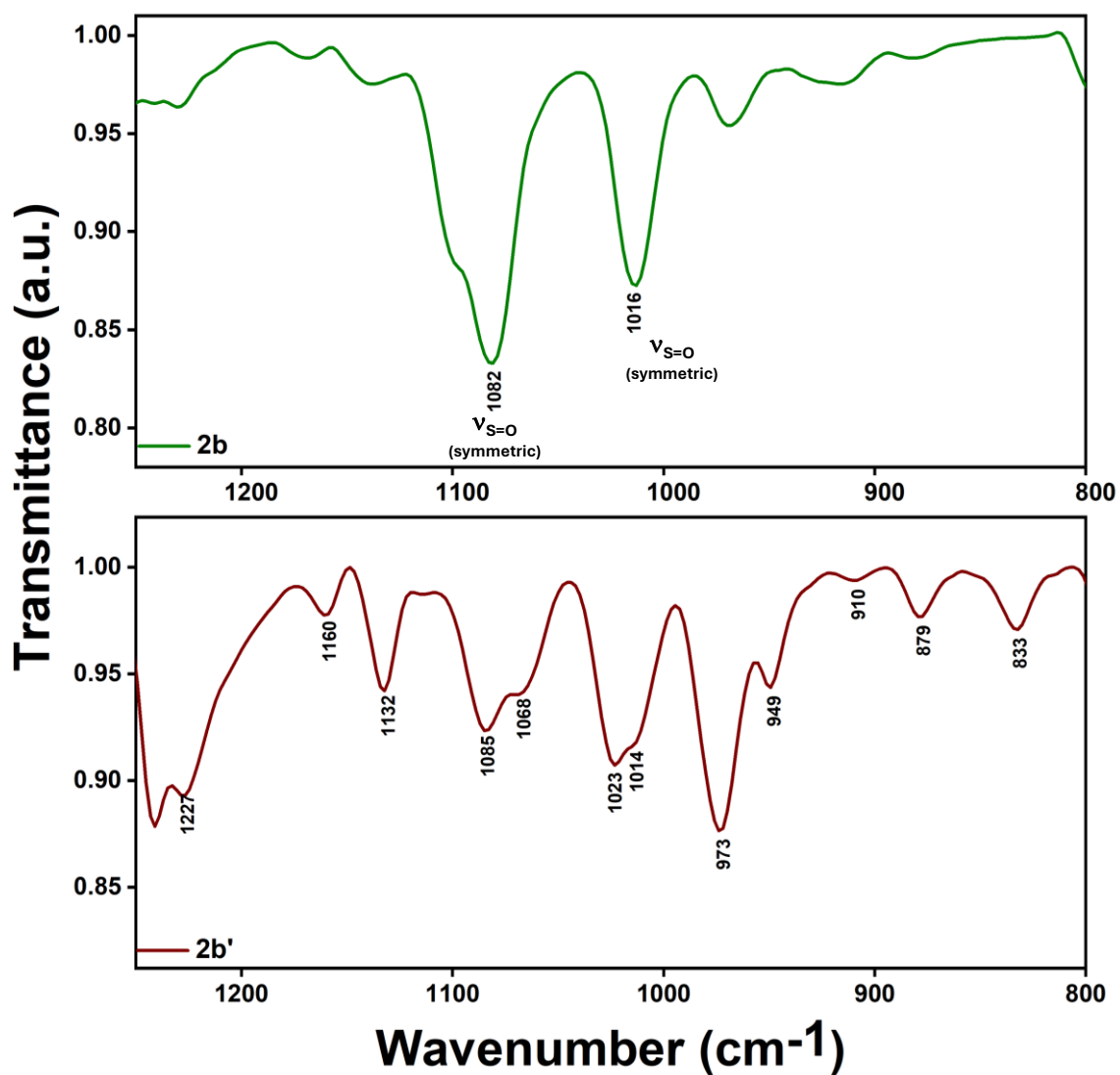
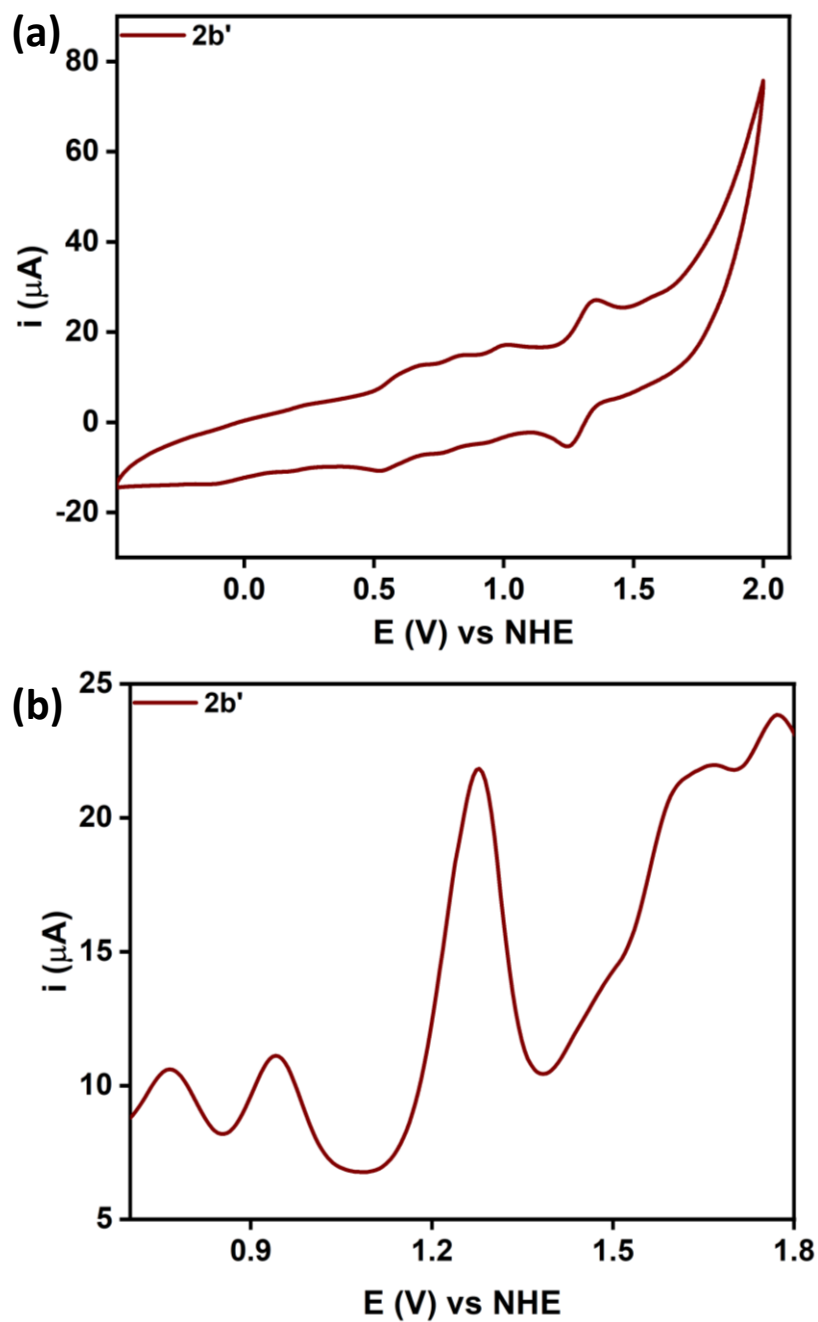


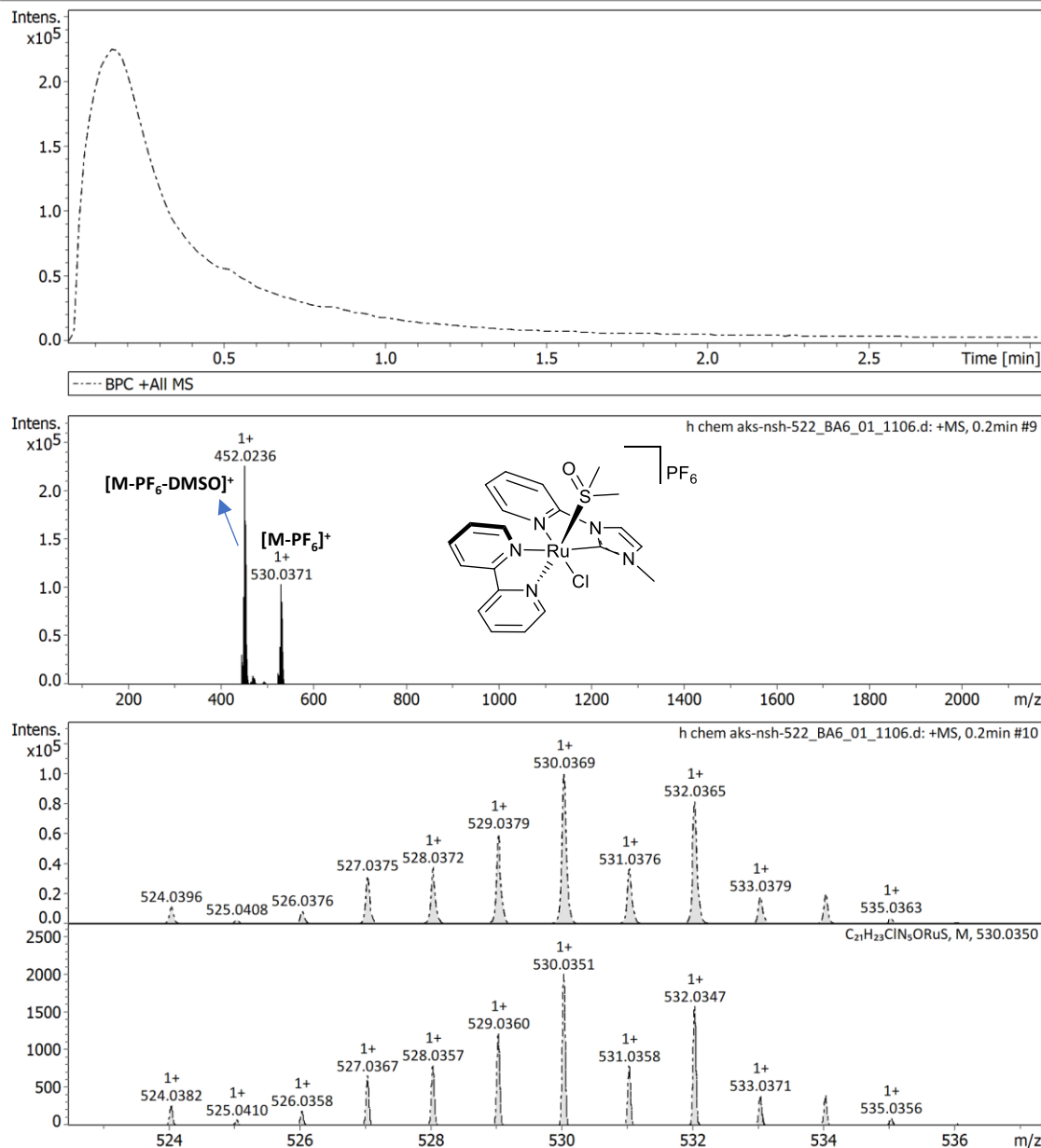
Figure S15. Comparative IR spectra of **2b** (up) and **2b'** (down) for the



**Figure S16.** (a) Cyclic voltammogram and (b) DPV of complex **2b'** recorded in  $\text{CH}_2\text{Cl}_2$  using 0.1 M  $\text{NH}_4\text{PF}_6$  as the supporting electrolyte.

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**Figure S17.** LCMS and HRMS of complex **3a**.

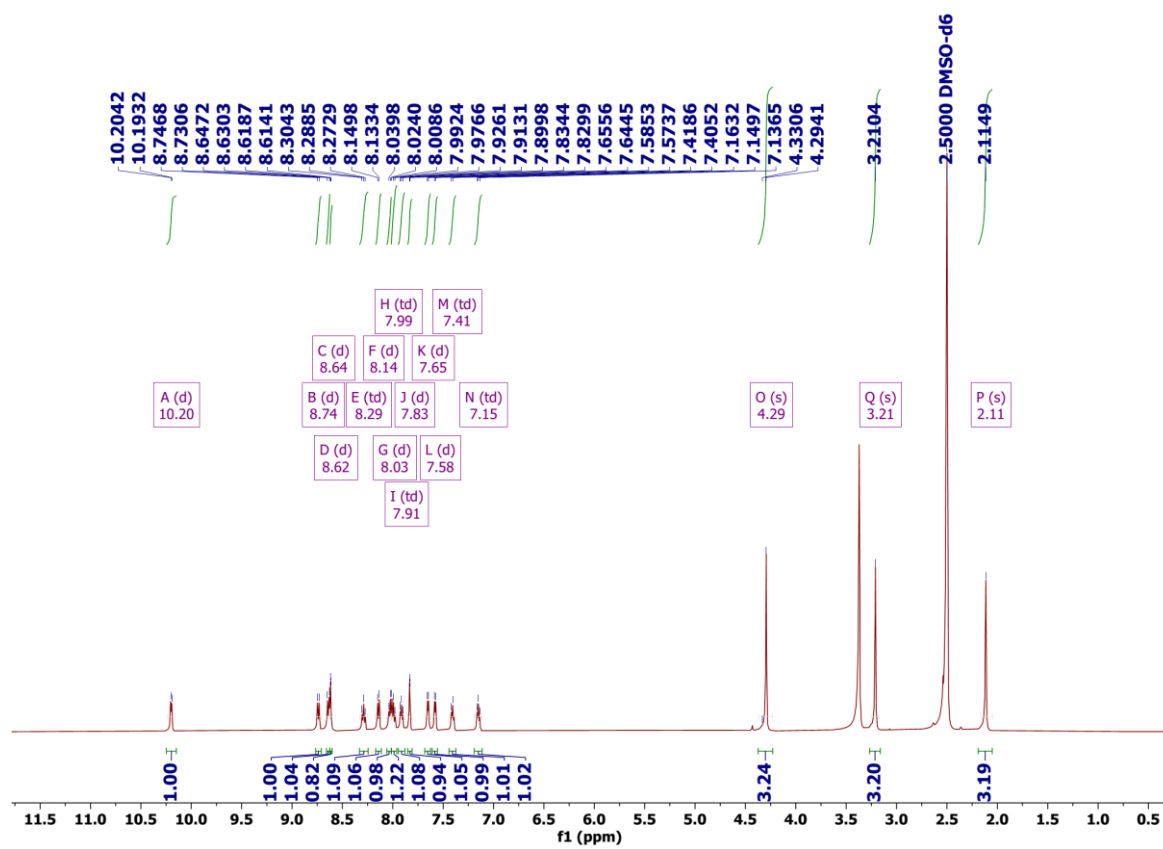


Figure S18.  $^1\text{H}$  NMR of complex **3a** recorded in DMSO- $\text{d}_6$ .

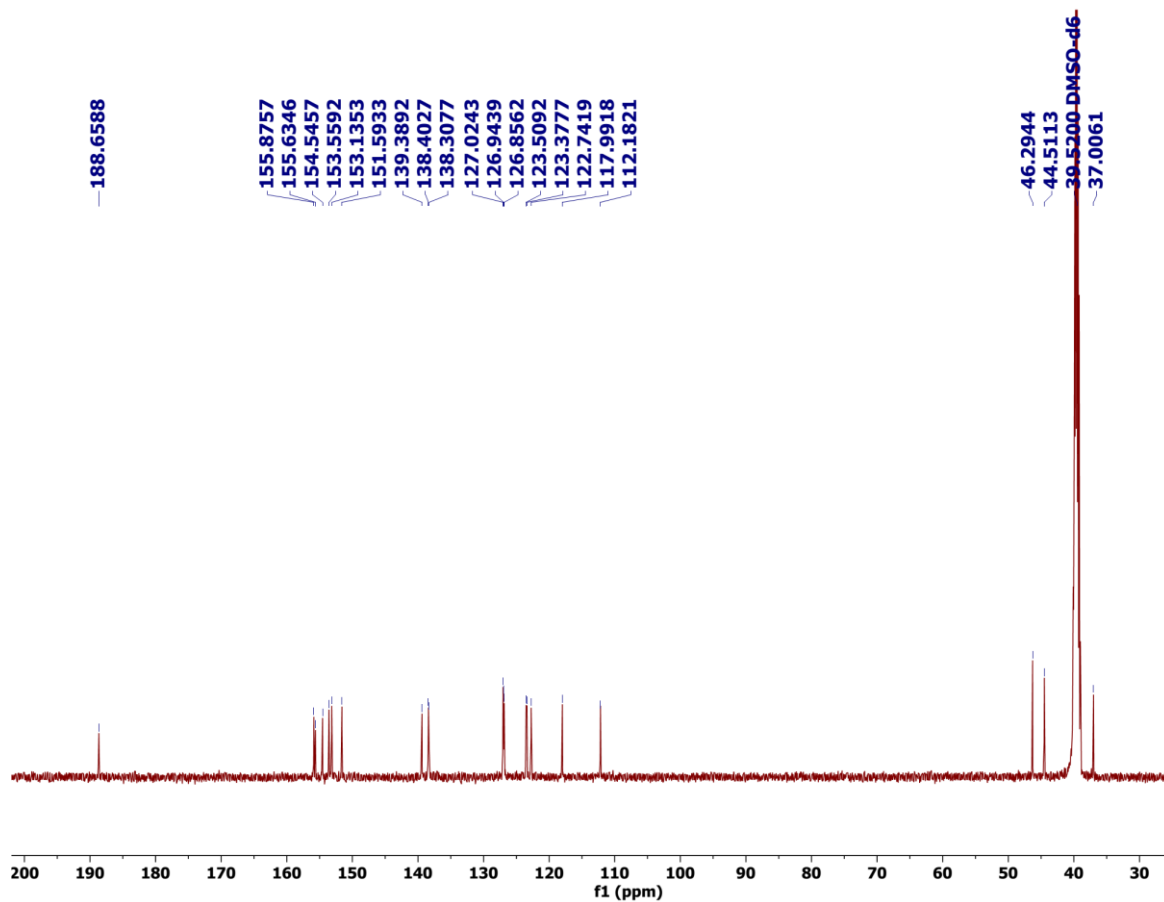
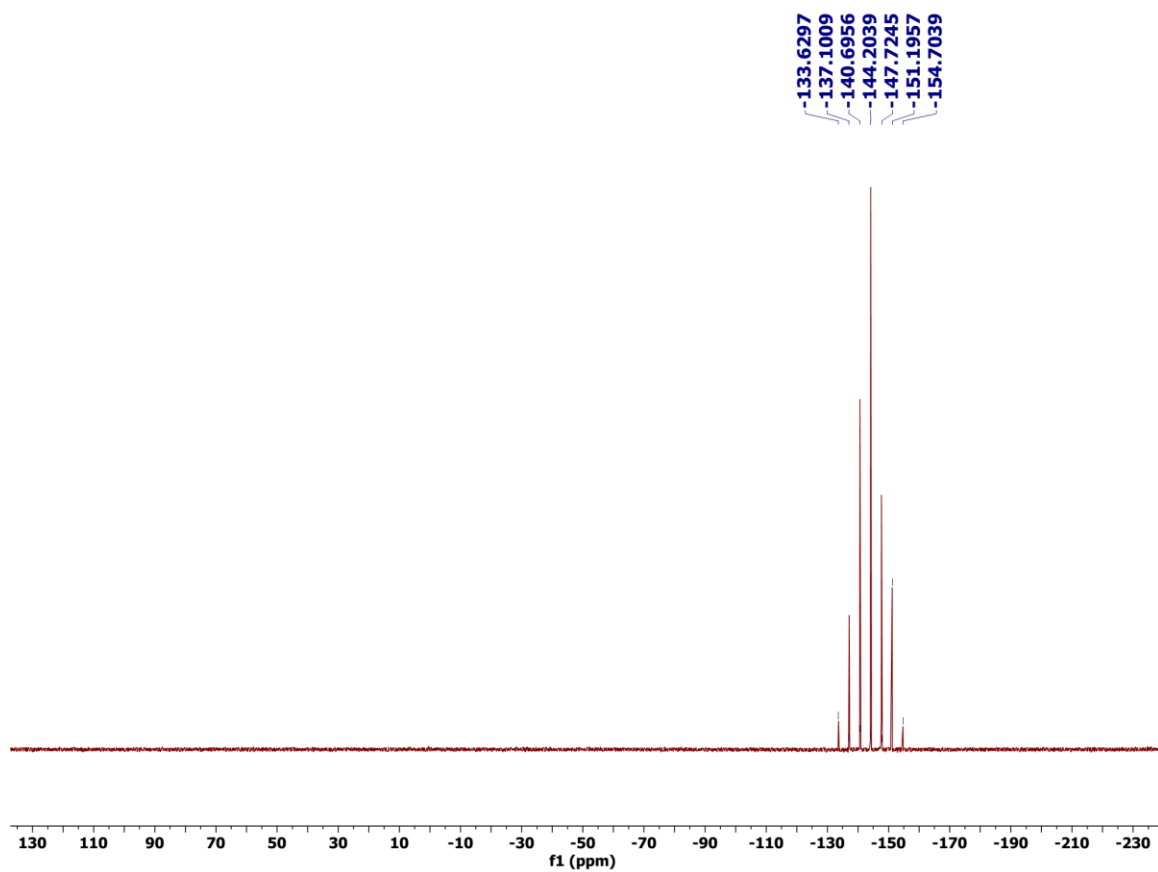


Figure S19.  $^{13}\text{C}$  NMR of complex **3a** recorded in DMSO- $\text{d}_6$ .



**Figure S20.**  $^{31}\text{P}$  NMR of complex **3a** recorded in  $\text{DMSO-d}_6$ .



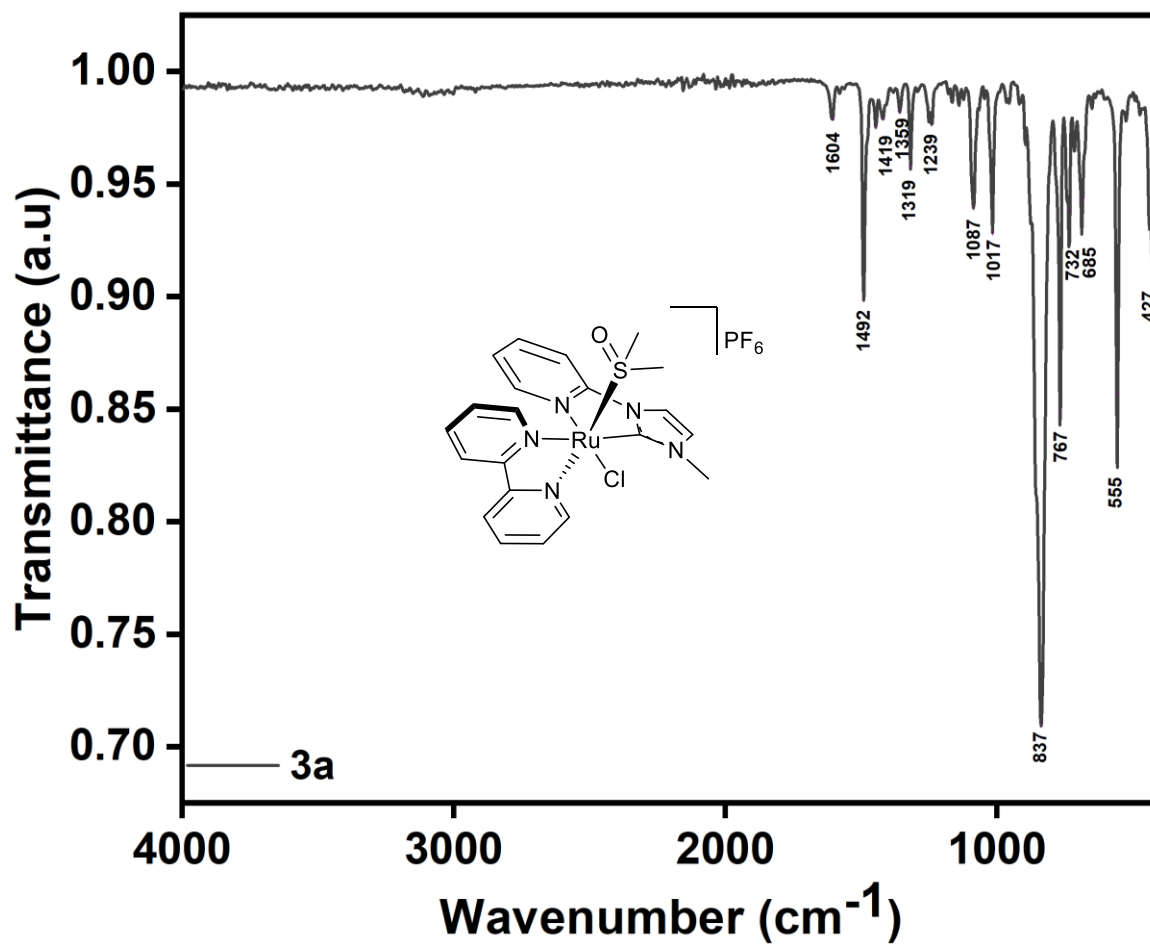
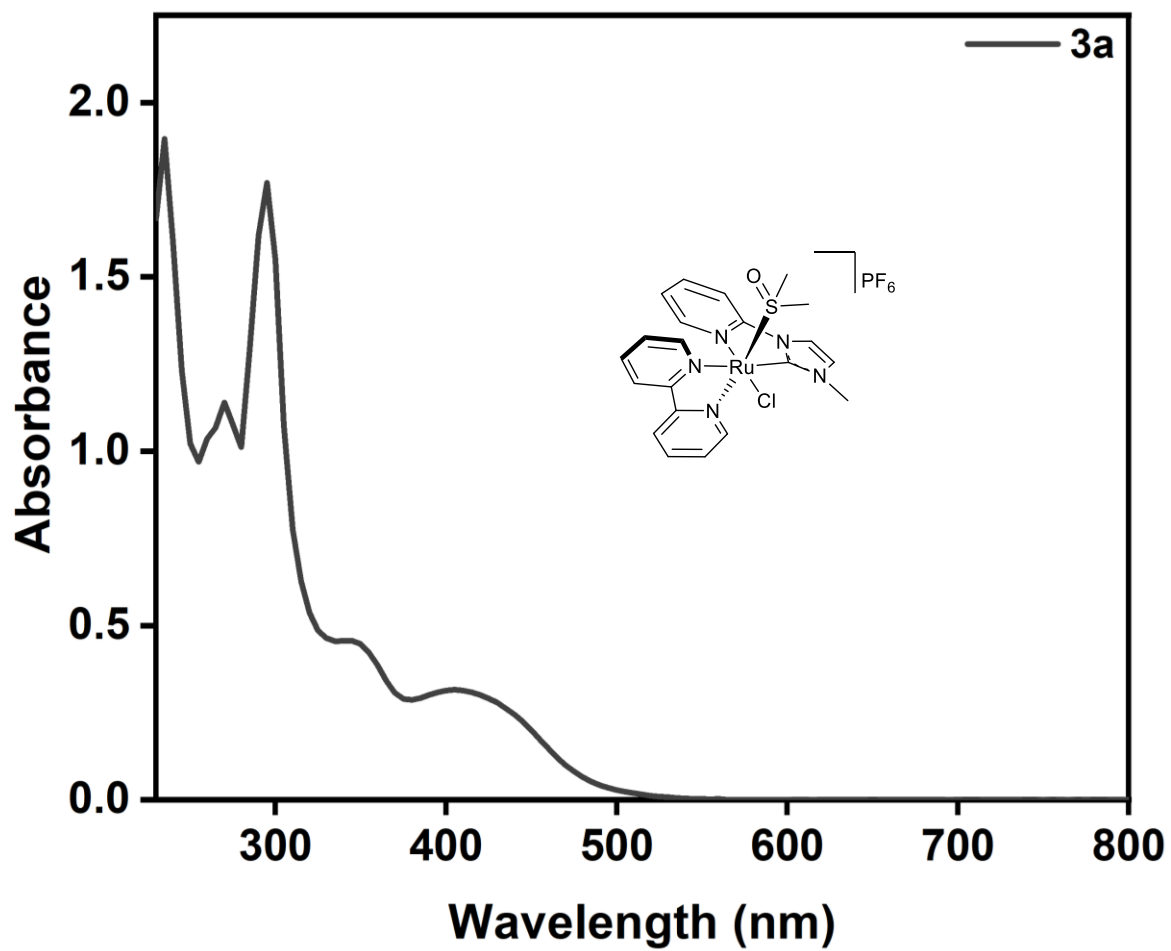


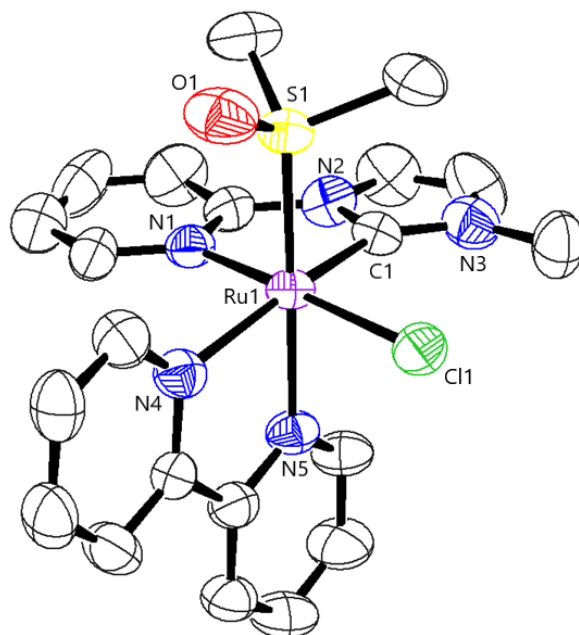
Figure S21. IR spectrum of complex **3a** in solid state.



**Figure S22.** UV-Vis spectrum of complex **3a** recorded in MeOH at room temperature.

### Description of crystal structure of **3a**

The X-ray quality crystals of complex **3a** have been obtained by the slow diffusion of diethyl ether into the methanolic solution of the complex at 4 °C. The complex **3a** is crystallized in triclinic crystal system with the space group *P*-1. Asymmetric crystal lattice contains two molecules of the complex. The coordination sphere consists of the bidentate ligand scaffold, N^N cyclometalated 2,2'-bipyridine, one DMSO and one chloride ligand arranged in a pseudo-octahedral fashion. The bite angle for the N1-Ru1-C1 was found be 78.2(5) ° which is slightly smaller than the bite angle observed in **2a**, however falls in the range reported for the Ru(II)-NHC complexes. The Ru1-C1 (2.009 Å) bond distance reveals close similarity with the complexes reported in literature. Furthermore, it is interesting to note that the shortening of the Ru1-S1 bond distance from 2.3021(18)Å (in **2a**) to 2.269(3)Å (in **3a**) can be attributed to the better  $\sigma$ -donor and  $\pi$ -acceptor properties of the bpy ligand compared to the  $\pi$ -donor chloride ligand in **2a**. Moreover, the slight hydrogen bonding interaction between O<sub>DMSO</sub>...H<sub>py</sub> trans to carbene was observed, which might have restricted the Ru-S single bond rotation. It is concomitant with the two different resonances observed in <sup>1</sup>H and <sup>13</sup>C NMR data for the two distinct -CH<sub>3</sub> groups of the DMSO ligand. All other bond distances and bond angles were found to be in accordance with the literature reports and listed in table S3-S4.



**Figure S23.** ORTEP diagrams for complex **3a** obtained from X-ray diffraction. Hydrogen atoms and counterion ( $\text{PF}_6^-$ ) are excluded for clarity. Ellipsoids are shown at the 50% probability level. Selected bond distances(Å) and bond angles(°) are Ru1-C1 2.009(12); Ru1-N1 2.064(10); Ru1-S1 2.269(3); Ru1-Cl1 2.418(3); Ru1-N4 2.150(11); Ru1-N5 2.108(10); C1-Ru1-N1 78.2(5); and C1-Ru1-N4 168.7(4).

## Generic Display Report

### Analysis Info

Analysis Name	F:\Project 4\OneDrive_2023-09-08\h chem aks-nsh-1b-db_RD1_01_2618.d	Acquisition Date	08-09-2023 16:55:18
Method	8. LCMS tune wide MeOH.m	Operator	Ghanashyam
Sample Name	h chem aks-nsh-1b-db	Instrument	micrOTOF-Q
Comment			

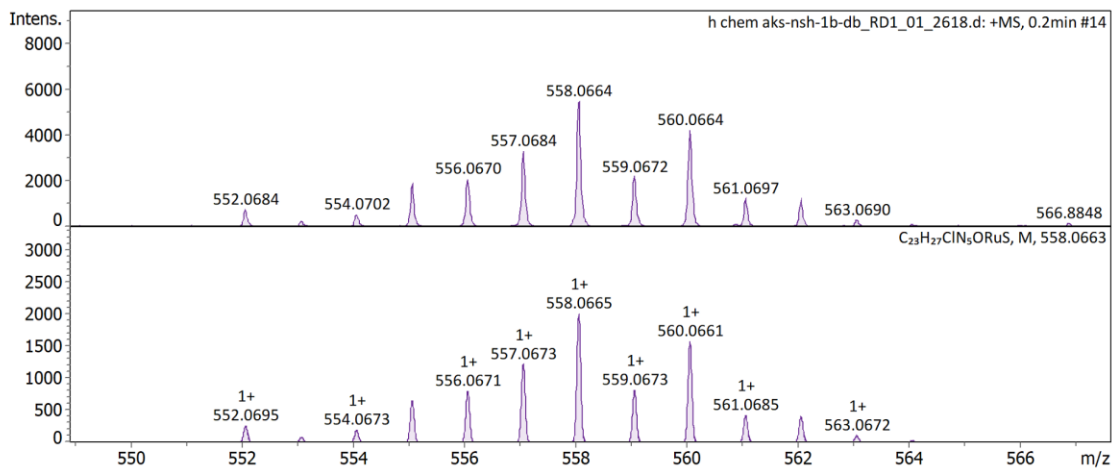
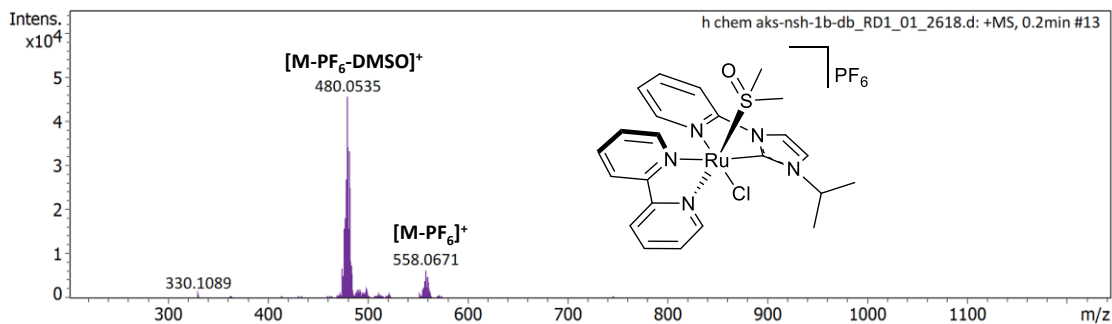
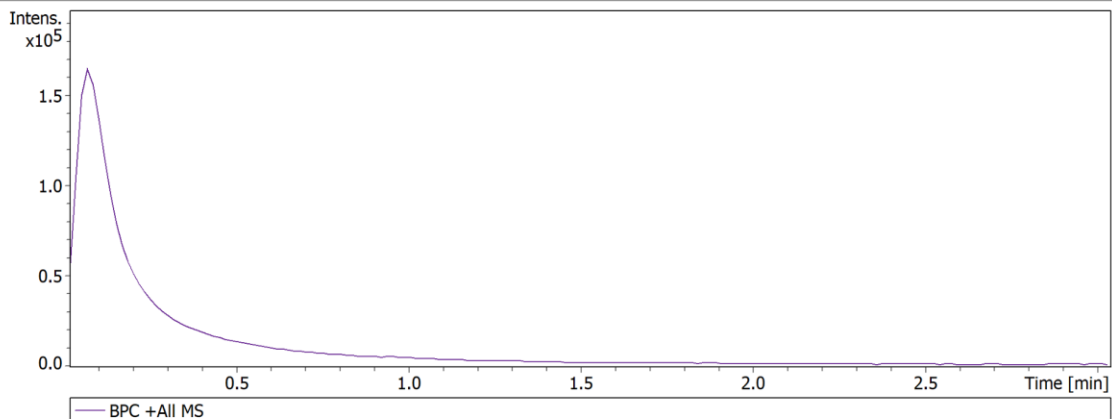


Figure S24. LCMS and HRMS of complex **3b**.

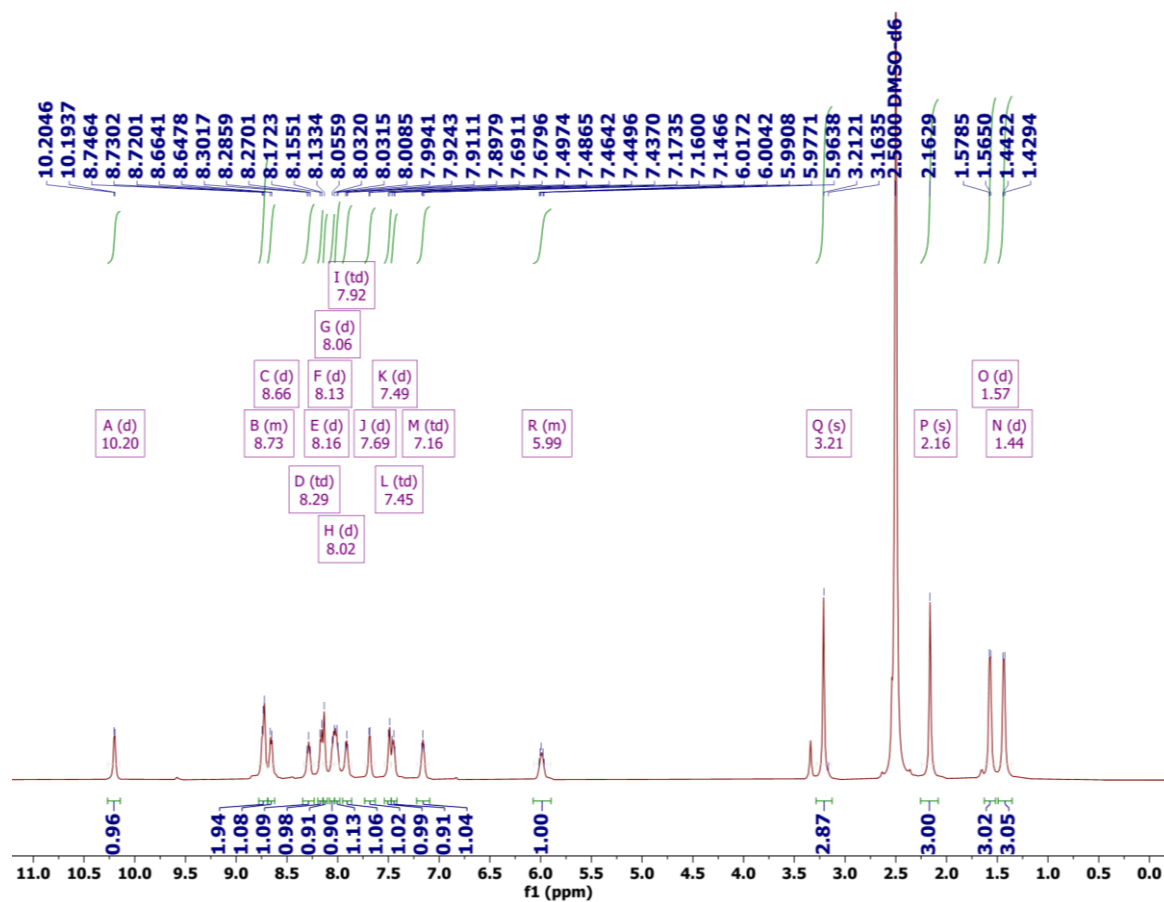
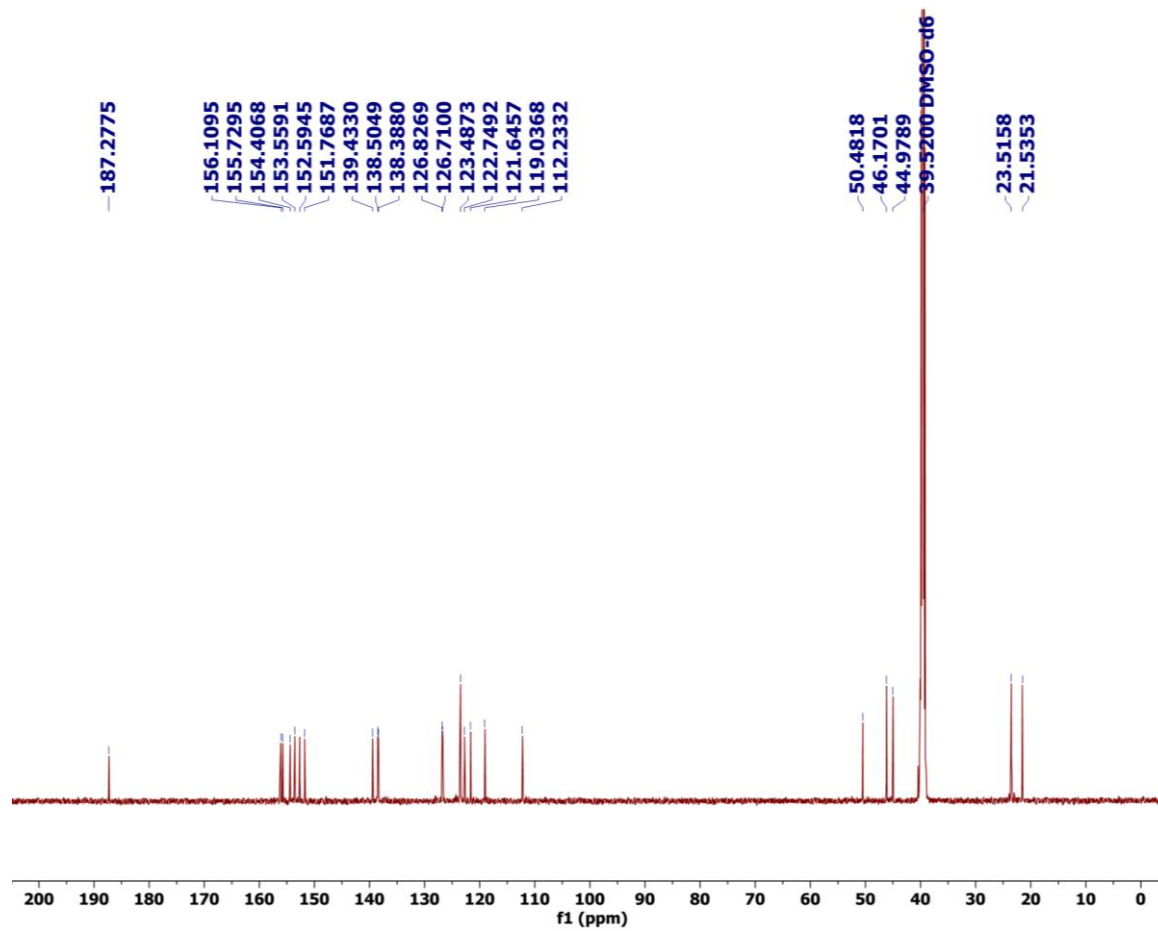
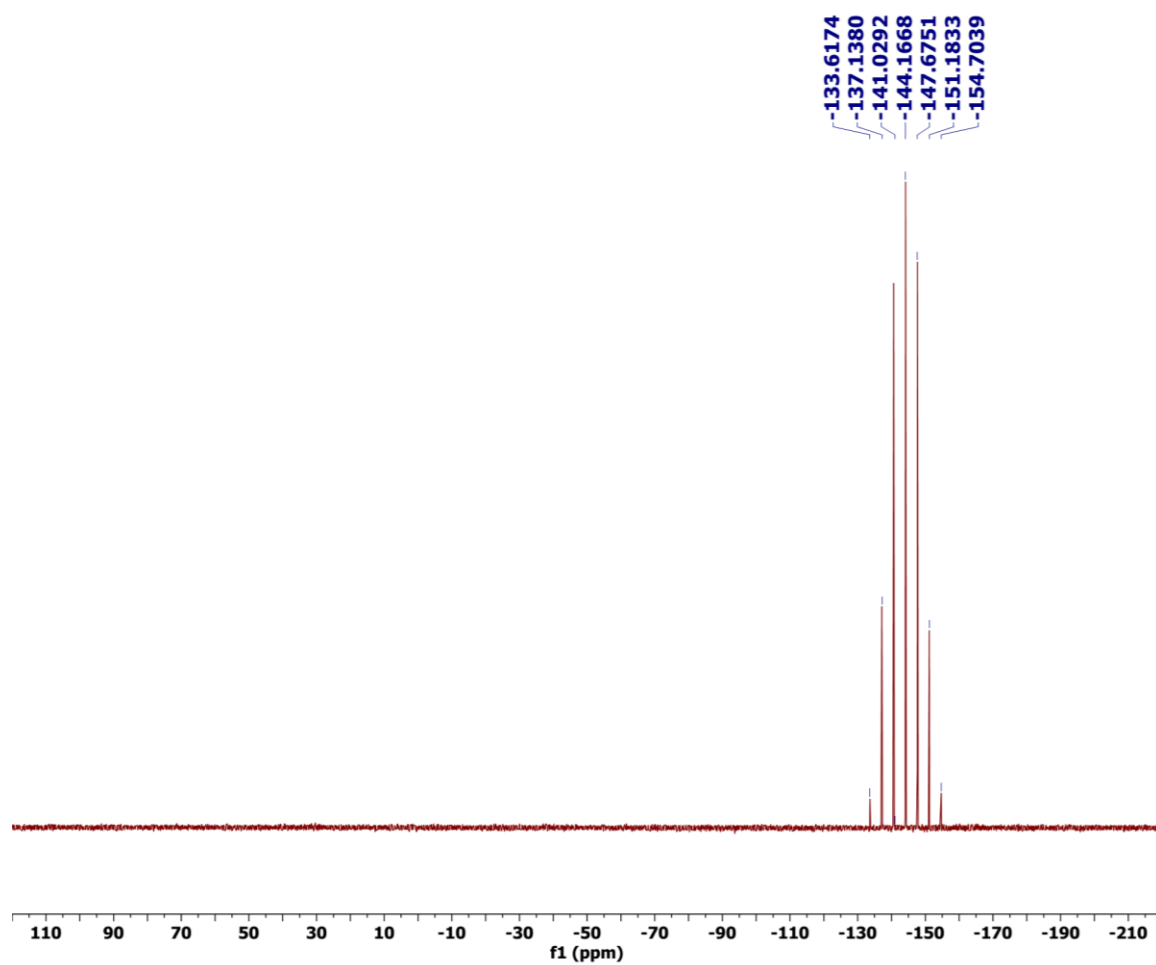


Figure S25.  $^1\text{H}$  NMR of complex **3b** recorded in DMSO- $d_6$ .



**Figure S26.** <sup>13</sup>C NMR of complex **3b** recorded in DMSO-d<sub>6</sub>.



**Figure S27.**  $^{31}\text{P}$  NMR of complex **3b** recorded in  $\text{DMSO-d}_6$ .

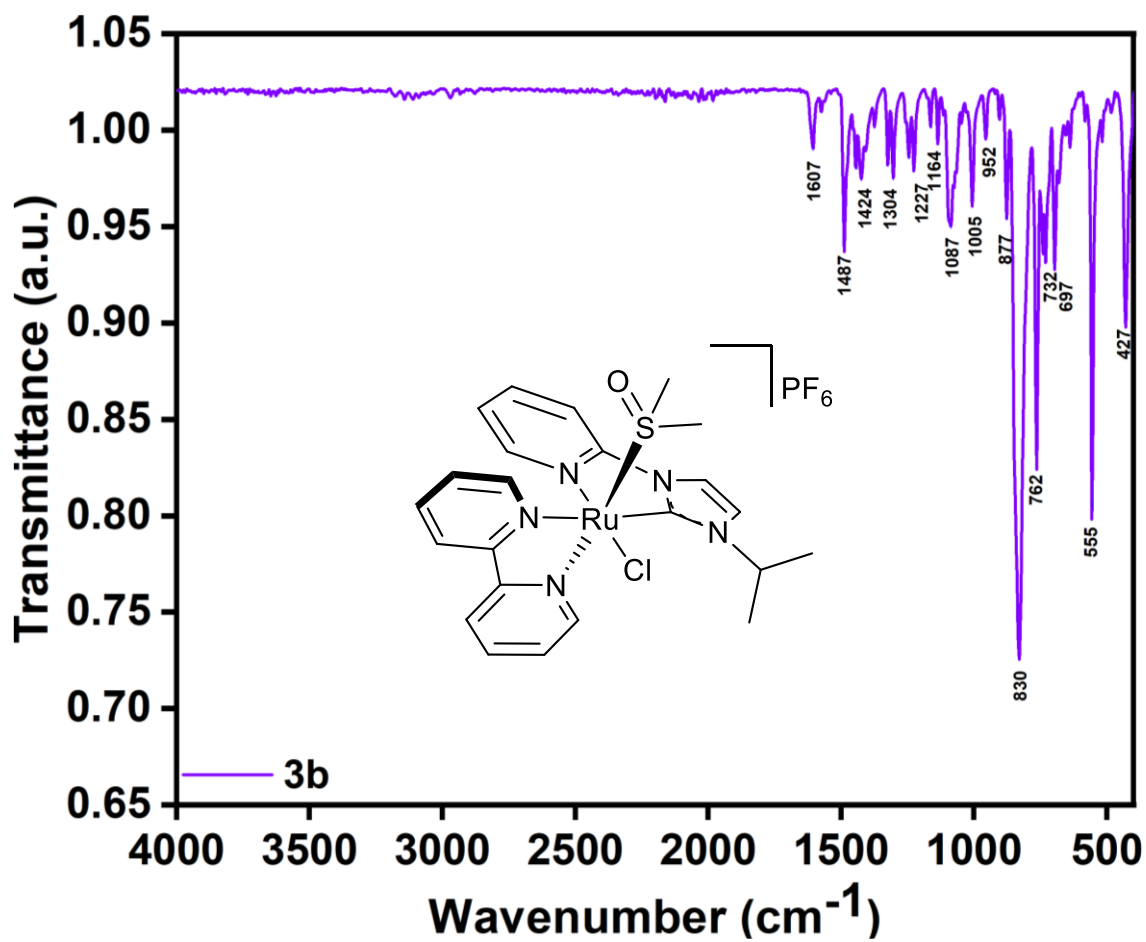
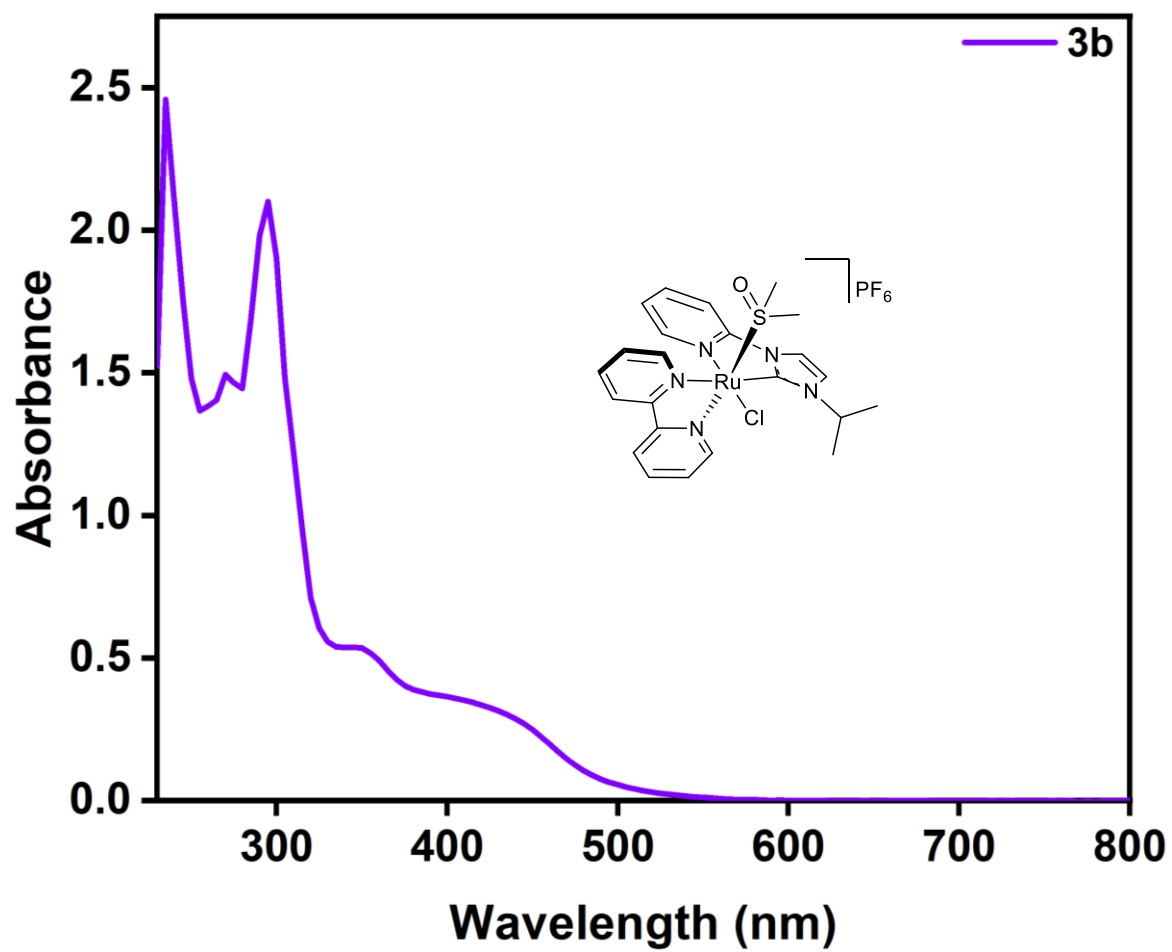
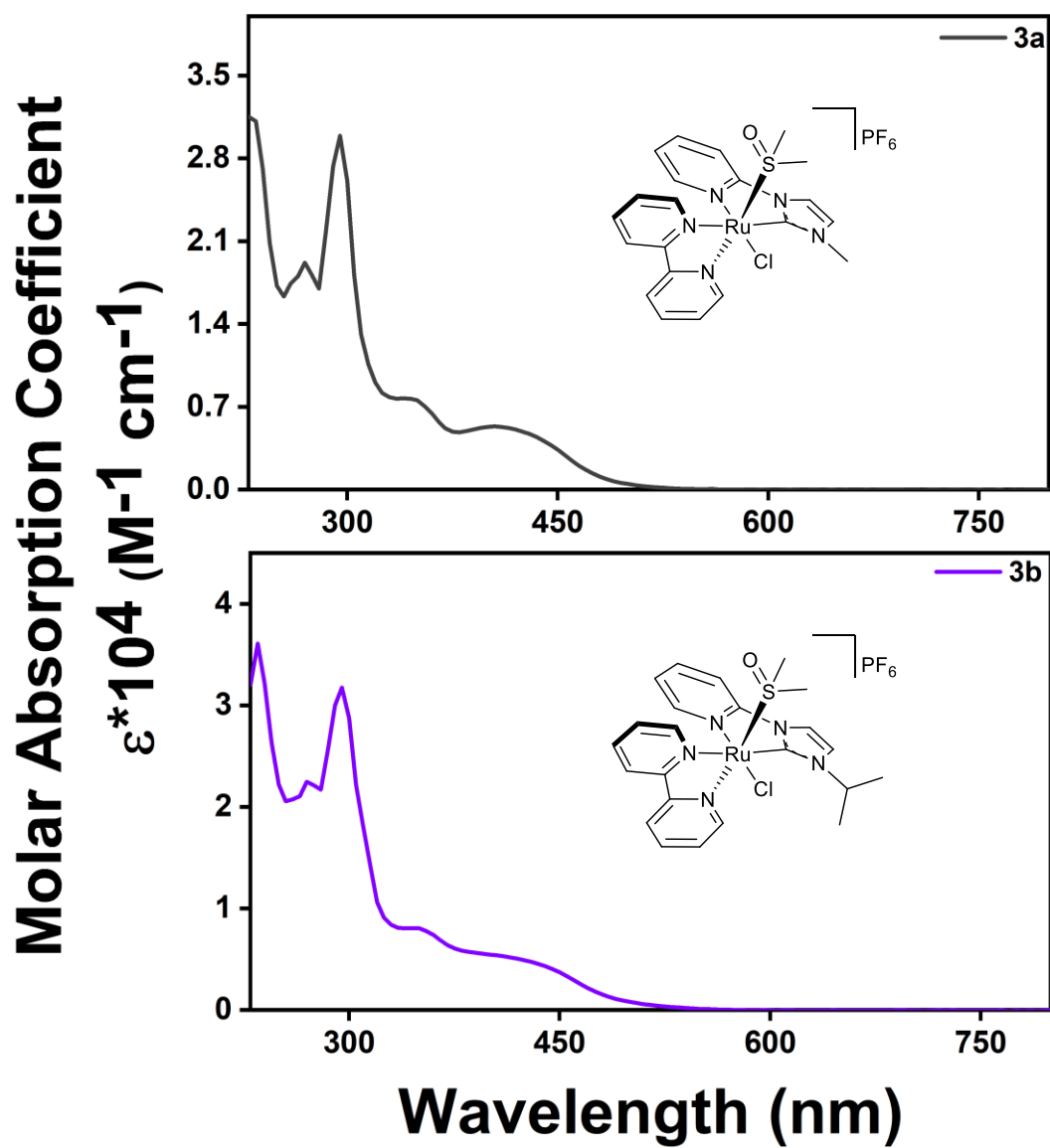


Figure S28. IR spectrum of complex **3b** in solid state.

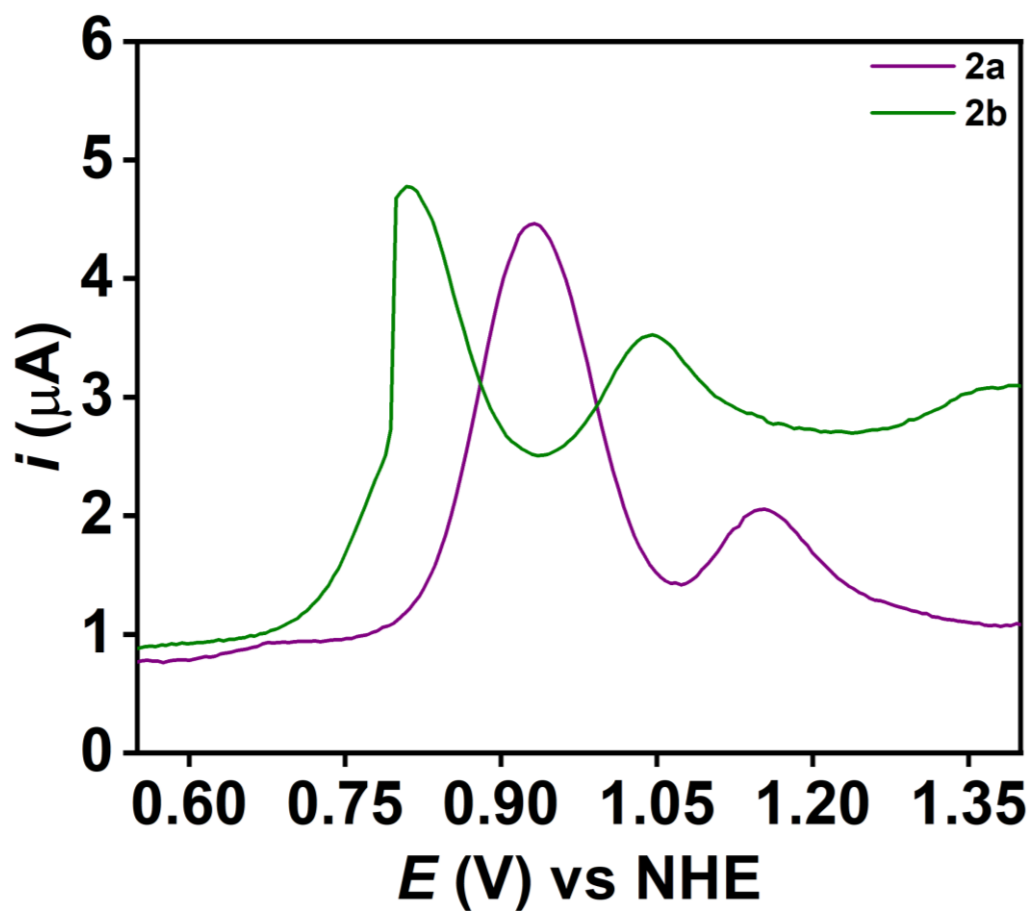




**Figure S29.** UV-Vis spectrum of complex **3b** recorded in MeOH at room temperature.



**Figure S30.** Stack plots of Molar absorption coefficients of complexes **3a** (up) and **3b** (down) recorded in DCM at room temperature.



**Figure S31.** Differential pulse voltammetry of complexes **2a** and **2b** recorded in  $\text{CH}_2\text{Cl}_2$  using 0.1 M TBAH as the supporting electrolyte.

**Table S1. Mathematical formulae used for the calculation of the equilibrium (K) and rate (k) constants.**

**Mathematical equations**

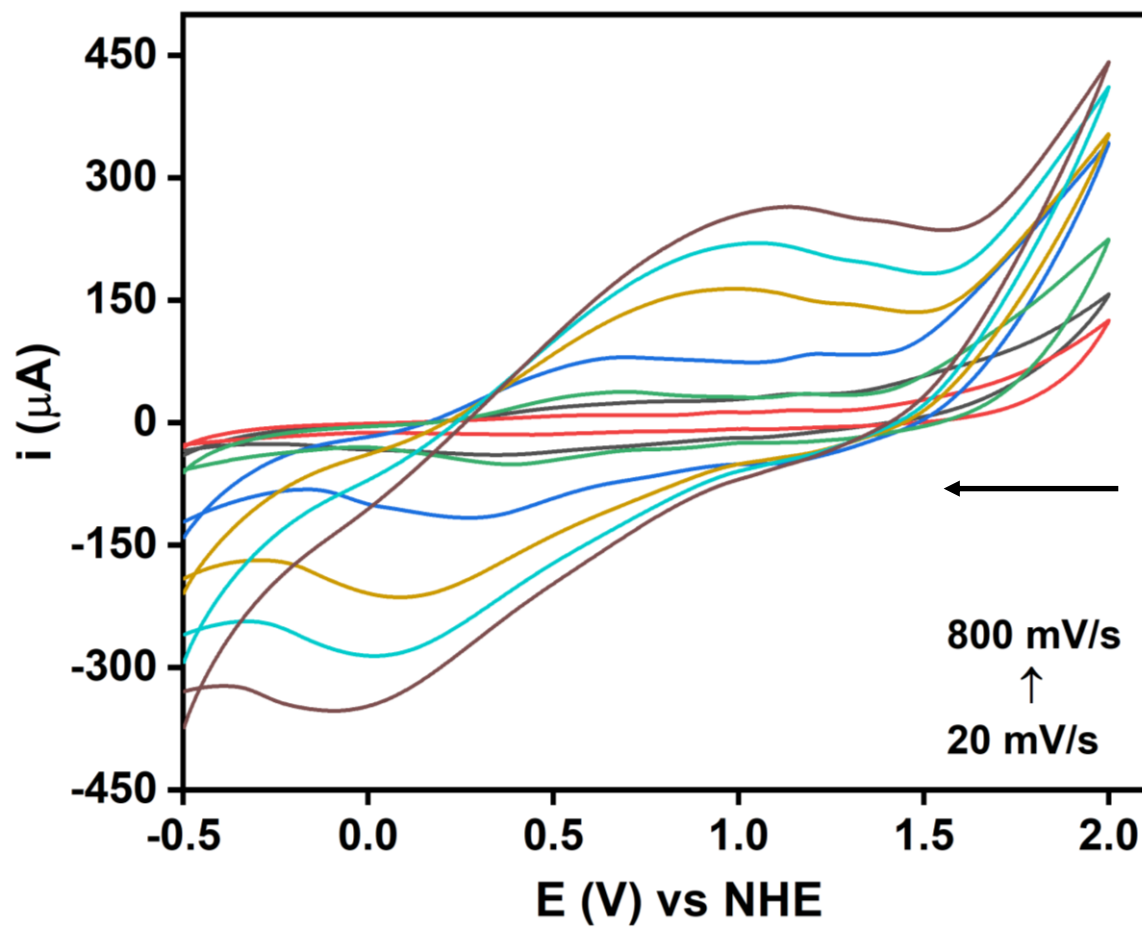
$$\frac{i_{c1}}{i_{c2}} = a \cdot \frac{1}{v} + K_{O-S}^{III} \quad (1)$$

$$\sqrt{v} = \frac{1}{\frac{0.471}{K_{O-S}^{III}} \cdot \sqrt{\frac{nFl}{RT}}} \cdot \frac{i_d}{i_k} - \frac{1.02}{\frac{0.471}{K_{O-S}^{III}} \cdot \sqrt{\frac{nFl}{RT}}} \quad (2)$$

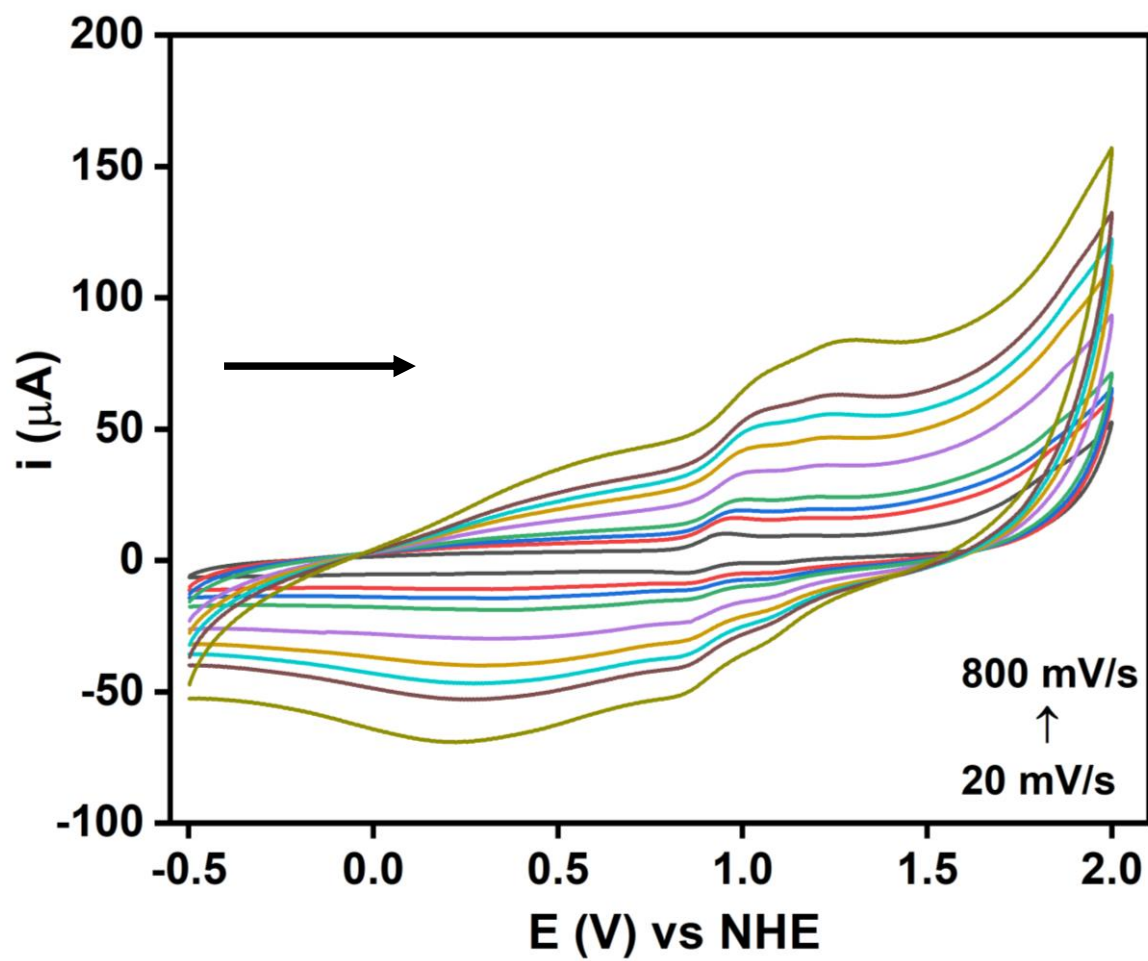
$$K^{II} = K^{III} + e^{\frac{F}{RT}(E_{Ru-S}^0 - E_{Ru-0}^0)} \quad (3)$$

$$\ln\left(\frac{i_{a1}}{\sqrt{v}}\right) = k_{\{O-S\}}^{II} \cdot \frac{1}{v} + b \quad (4)$$

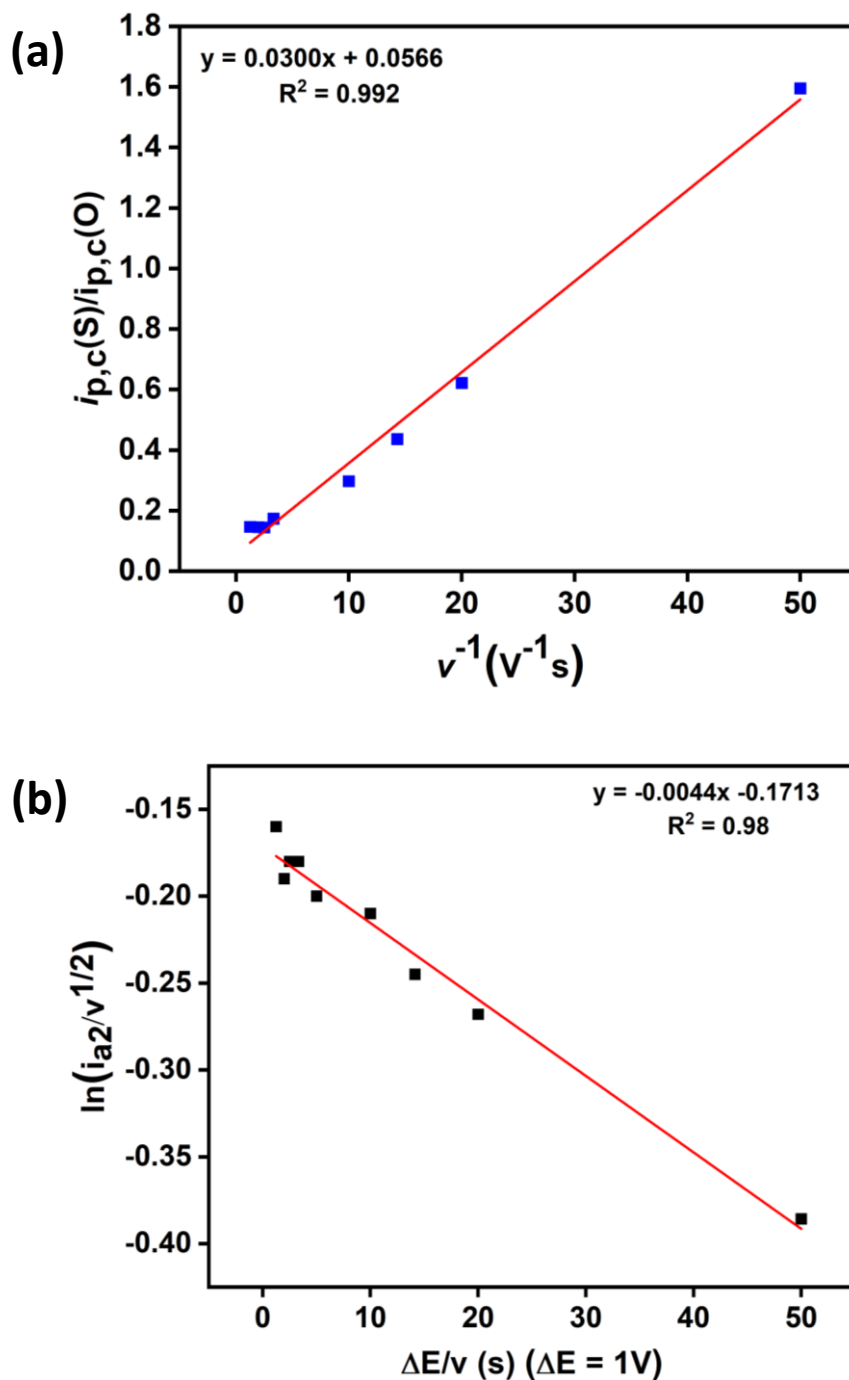
where,  $i_c$  = cathodic peak intensity (A),  $a = RT/nF$ , with:  $R$  = Boltzmann constant (J/(K·mol))  $T$  = temperature (K)  $n$  = number of exchanged electrons  $F$  = Faraday constant (A·s/mol)  $v$  = scan rate (V/s),  $K$  = equilibrium constant,  $i_a$  = diffusional current in the absence of a chemical reaction (=  $i_{a1}$ )  $i_k$  = measured peak current (=  $i_{c1}$ ),  $l = k_{O-S}^{III} + k_{S-O}^{III}$ ,  $E^\circ$  = standard potential.



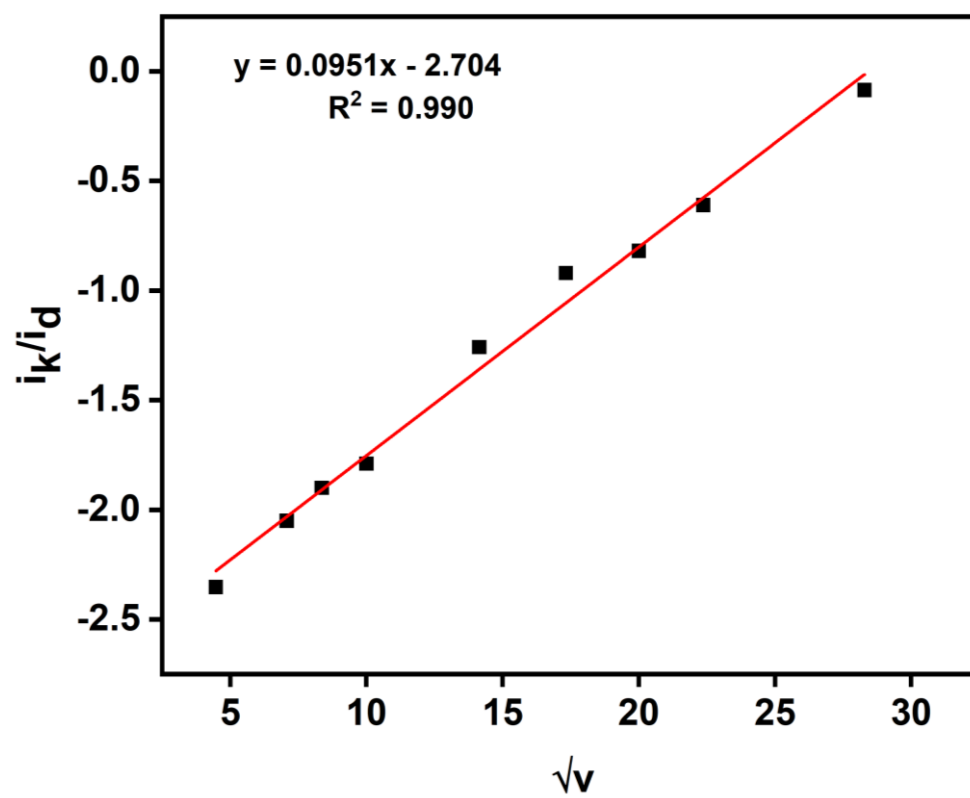
**Figure S32.** Cyclic voltammograms of **2a** in 0.1 M TBAH,  $\text{CH}_2\text{Cl}_2$ , at scan rates between 20 mV/s to 800 mV/s, after applying the CPE for 5 minutes at 2 V. Arrow indicates the starting potential and scanning direction.



**Figure S33.** Cyclic voltammograms of **2a** in 0.1 M TBAH,  $\text{CH}_2\text{Cl}_2$ , at scan rates between 20 mV/s to 800 mV/s, after applying the CPE for 5 minutes at -0.5 V. Arrow indicates the starting potential and scanning direction.

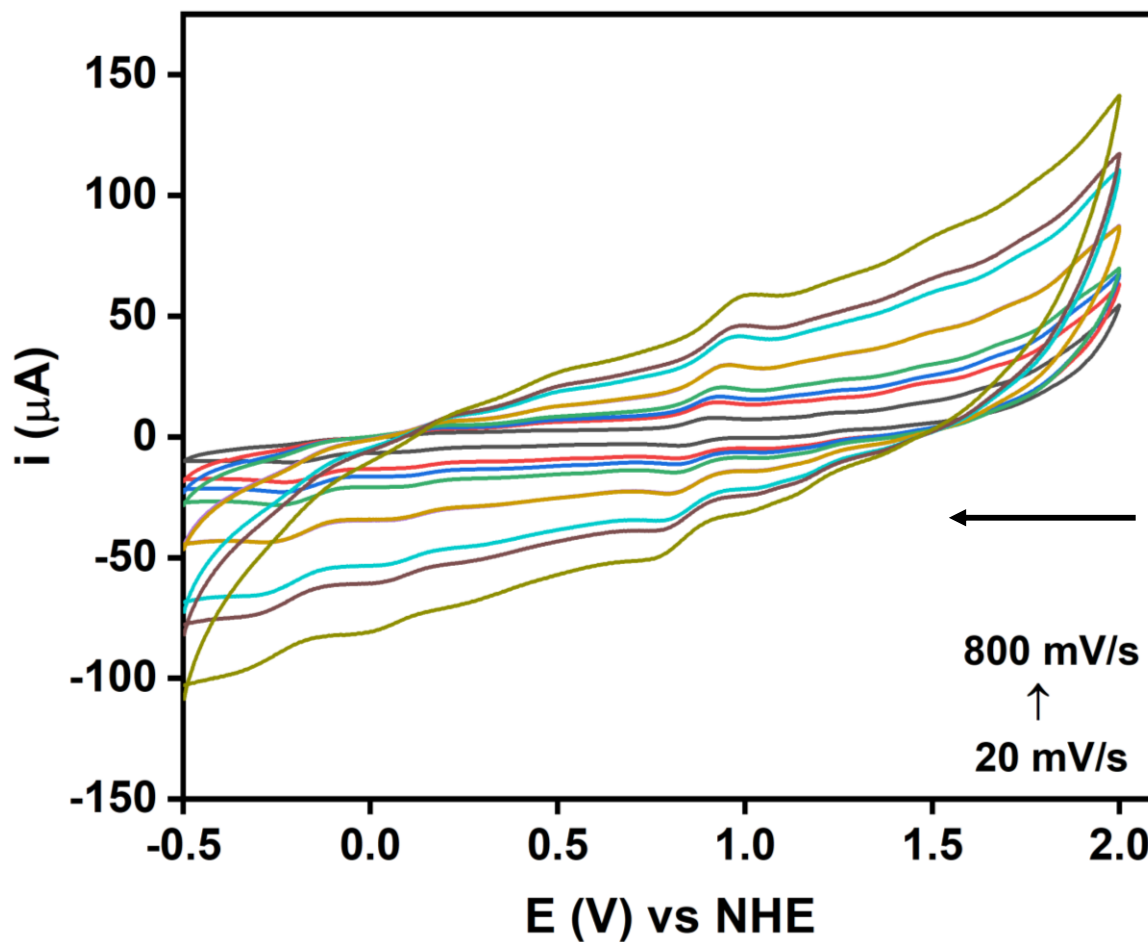


**Figure S34.** Plots of (a)  $i_{c1}/i_{c2}$  vs. inverse of the scan rate to obtain  $K^{III}_{O \rightarrow S}$  and (b)  $\ln(i_{a2}/\sqrt{v})$  vs. inverse of the scan rate to obtain  $k^{II}_{O \rightarrow S}$  for S-O linkage isomerization in complex **2a**.

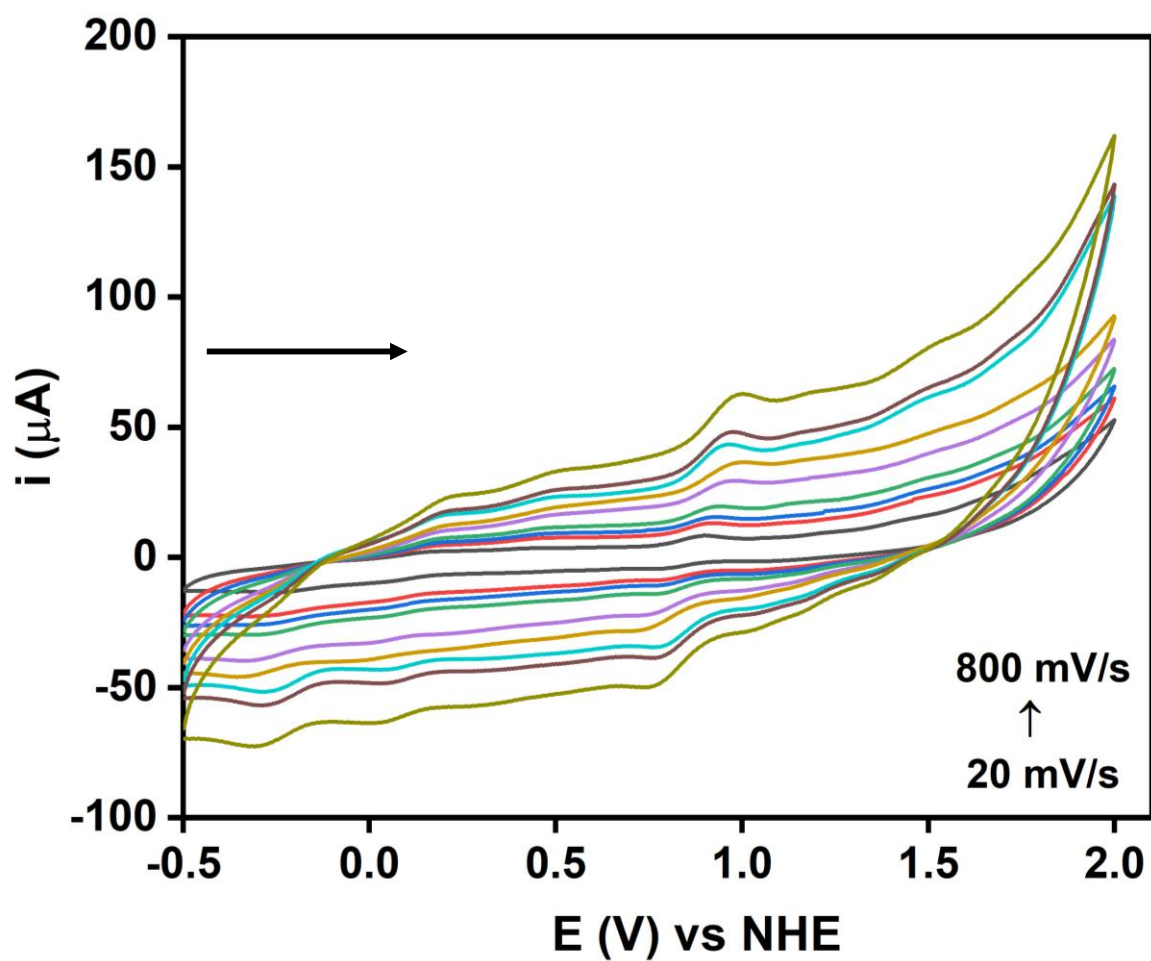


**Figure S35.** Plot of  $i_k/i_d$  vs.  $\sqrt{v}$  to obtain  $k_{S \rightarrow O}^{III}$  and  $k_{O \rightarrow S}^{III}$  for complex **2a**.

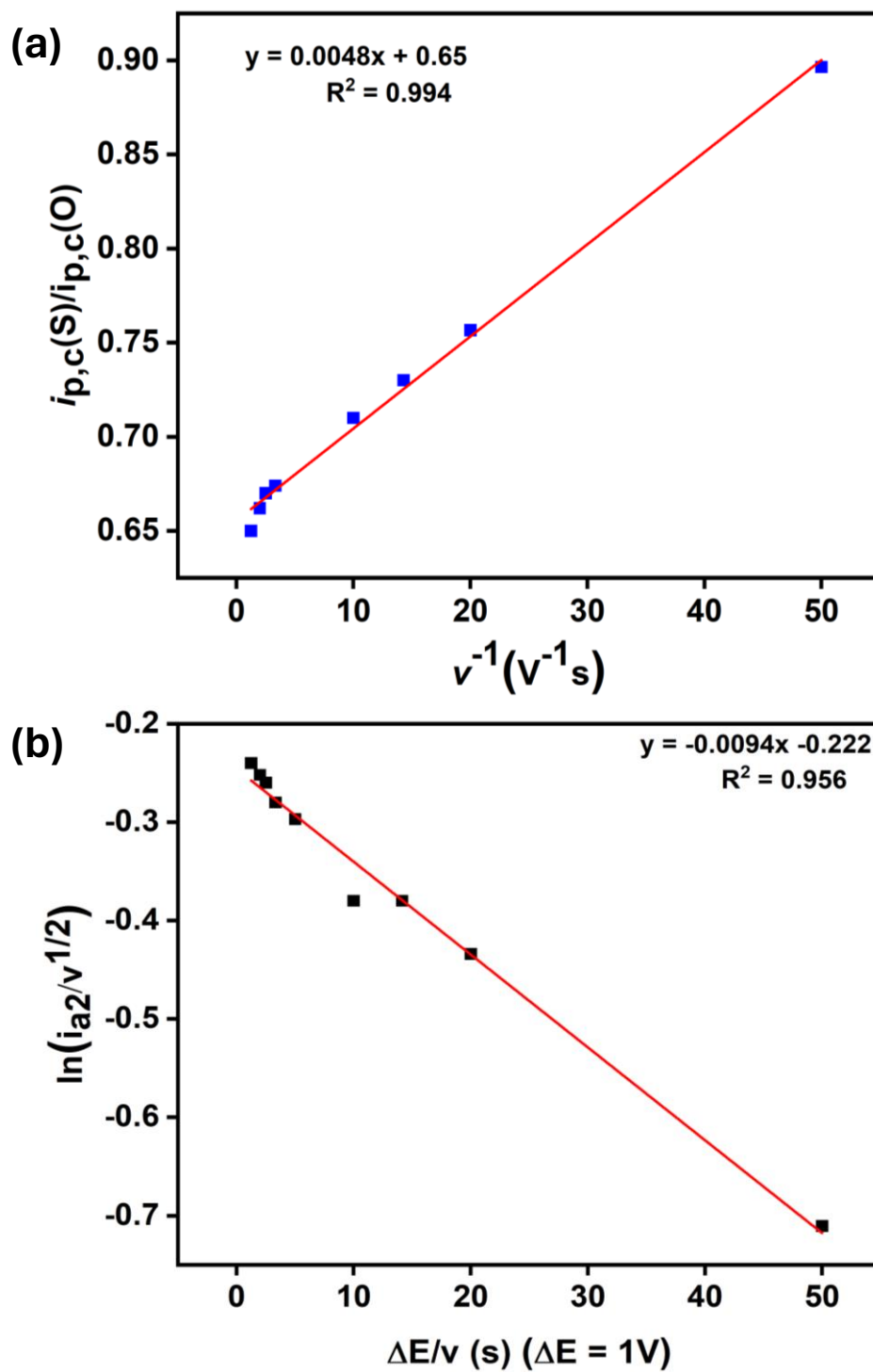




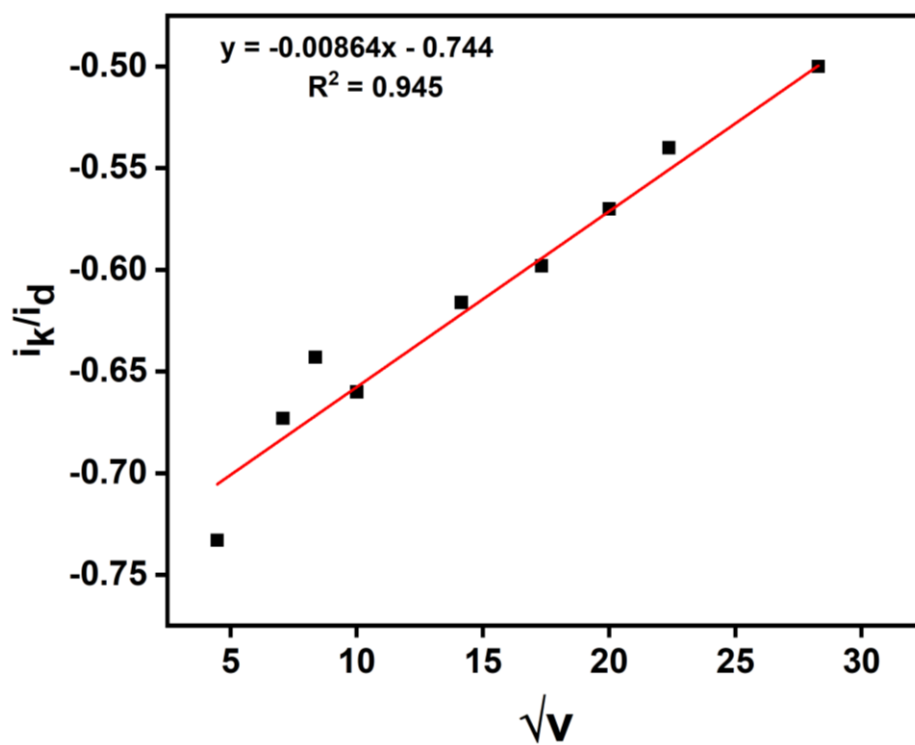
**Figure S36.** Cyclic voltammograms of **2b** in 0.1 M TBAH,  $\text{CH}_2\text{Cl}_2$ , at scan rates between 20 mV/s to 800 mV/s, after applying the CPE for 5 minutes at 2 V. Arrow indicates the starting potential and scanning direction.



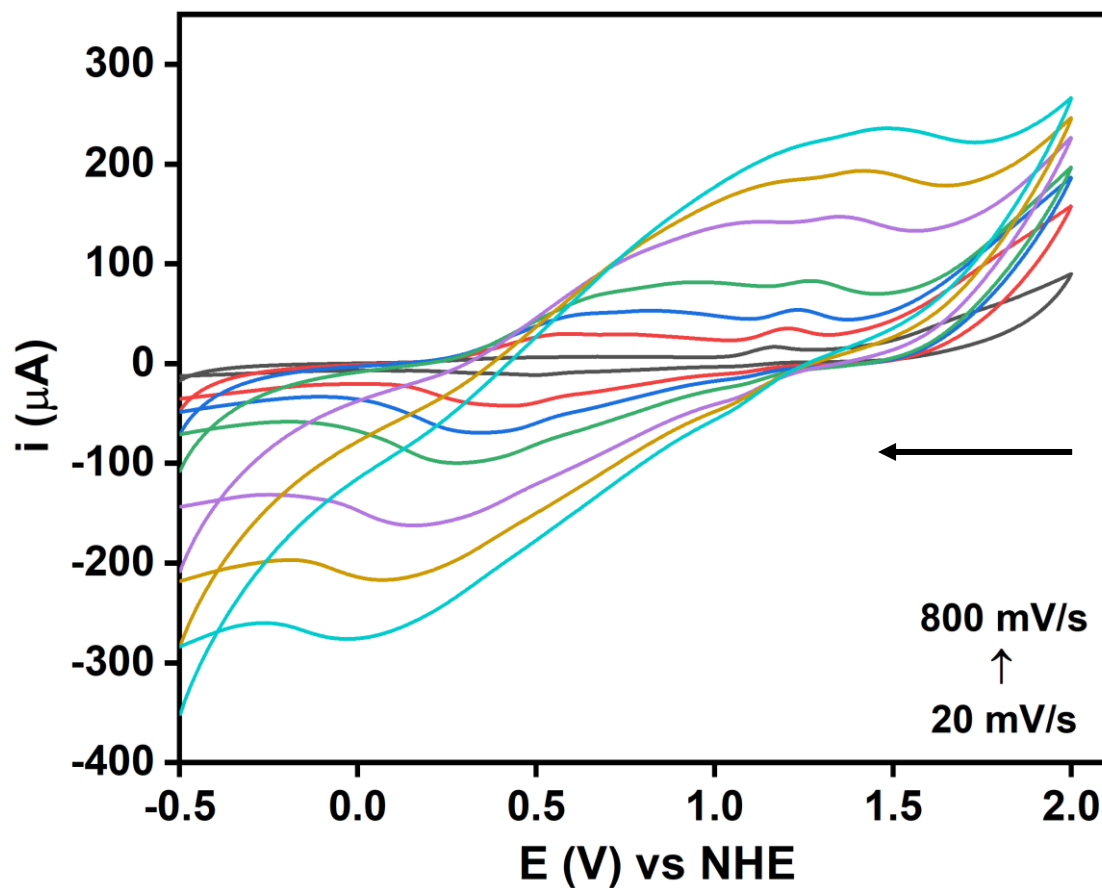
**Figure S37.** Cyclic voltammograms of **2b** in 0.1 M TBAH,  $\text{CH}_2\text{Cl}_2$ , at scan rates between 20 mV/s to 800 mV/s, after applying the CPE for 5 minutes at -0.5 V. Arrow indicates the starting potential and scanning direction.



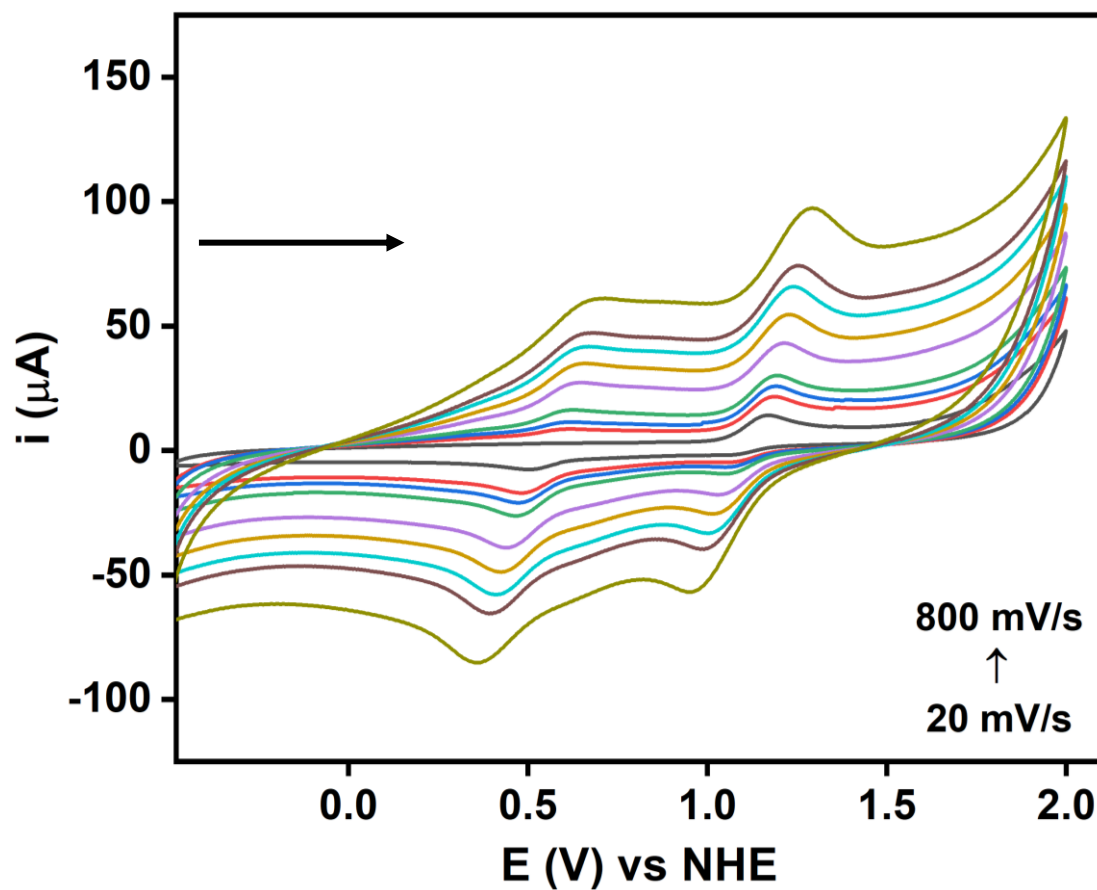
**Figure S38.** Plots of (a)  $i_{c1}/i_{c2}$  vs. inverse of the scan rate to obtain  $K^{III}_{O \rightarrow S}$  and (b)  $\ln(i_{a2}/\sqrt{v})$  vs. inverse of the scan rate to obtain  $k^{II}_{O \rightarrow S}$  for S-O linkage isomerization in complex **2b**.



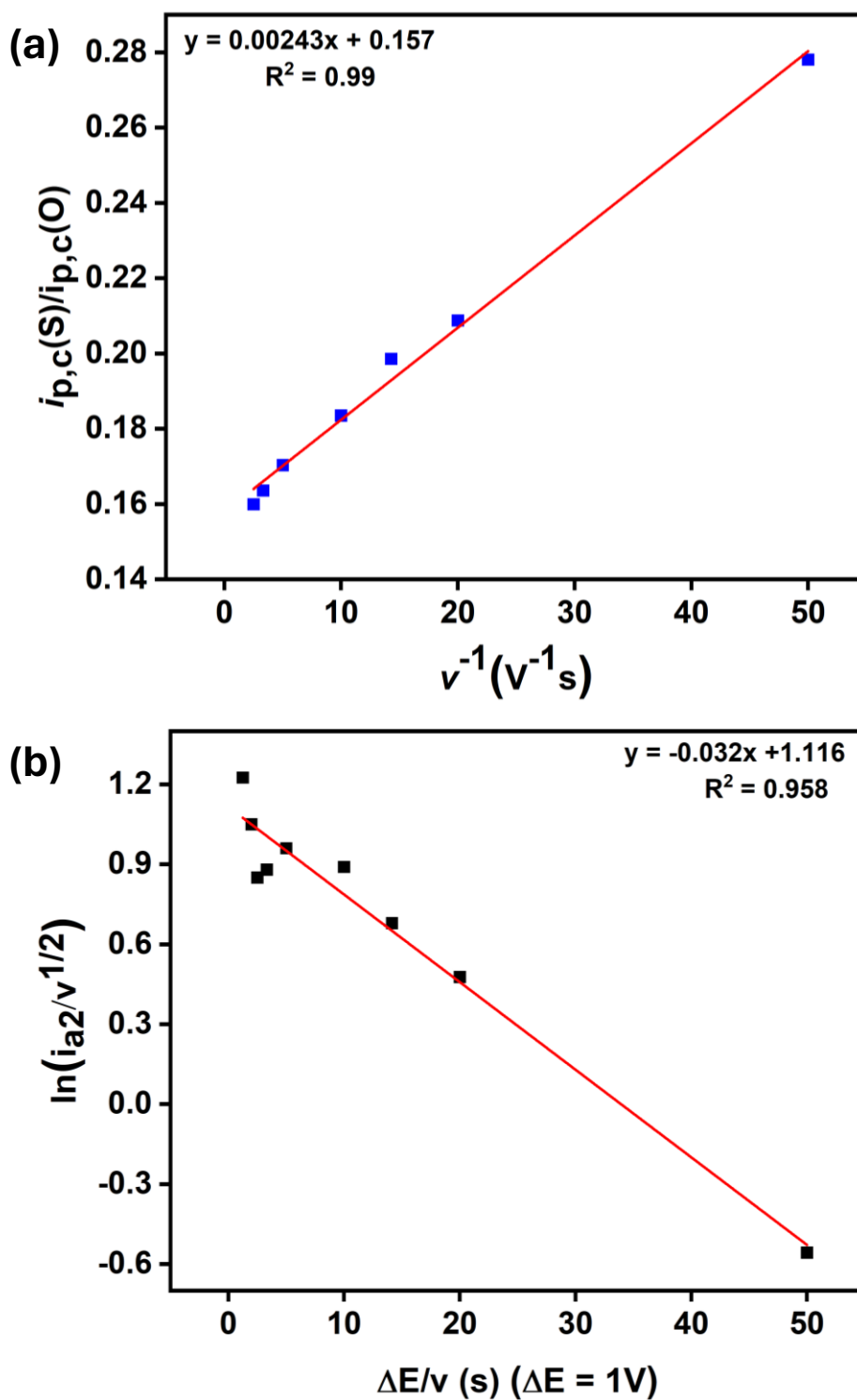
**Figure S39.** Plot of  $i_k/i_d$  vs.  $\sqrt{v}$  to obtain  $k_{S \rightarrow O}^{III}$  and  $k_{O \rightarrow S}^{III}$  for complex **2b**.



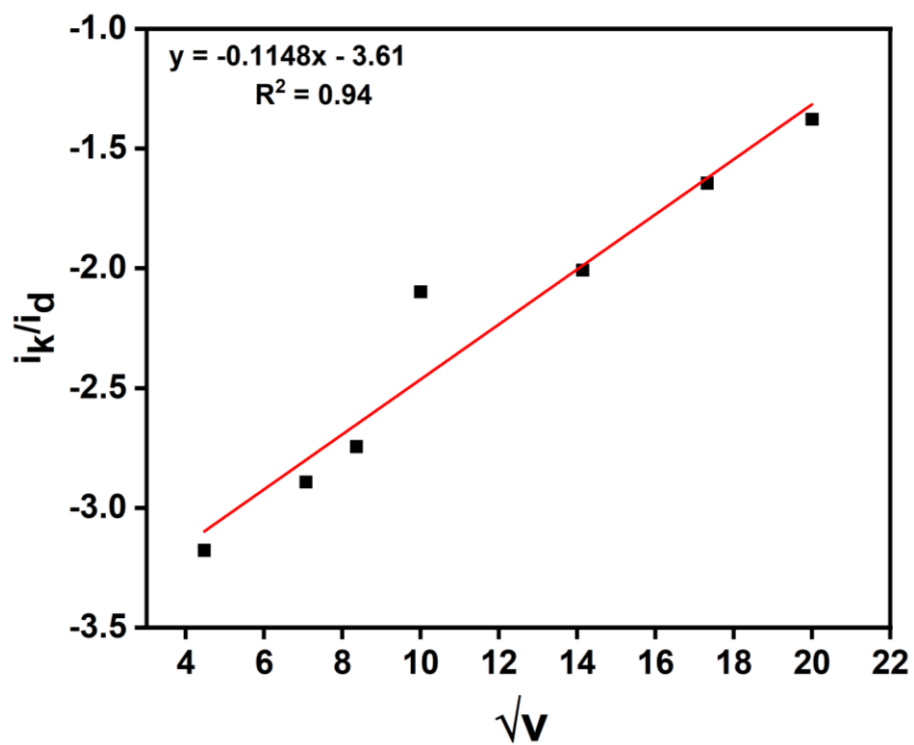
**Figure S40.** Cyclic voltammograms of **3a** in 0.1 M TBAH,  $\text{CH}_2\text{Cl}_2$ , at scan rates between 20  $\text{mV/s}$  to 800  $\text{mV/s}$ , after applying the CPE for 5 minutes at 2 V. Arrow indicates the starting potential and scanning direction.



**Figure S41.** Cyclic voltammograms of **3a** in 0.1 M TBAH,  $\text{CH}_2\text{Cl}_2$ , at scan rates between 20 mV/s to 800 mV/s, after applying the CPE for 5 minutes at -0.5 V. Arrow indicates the starting potential and scanning direction.

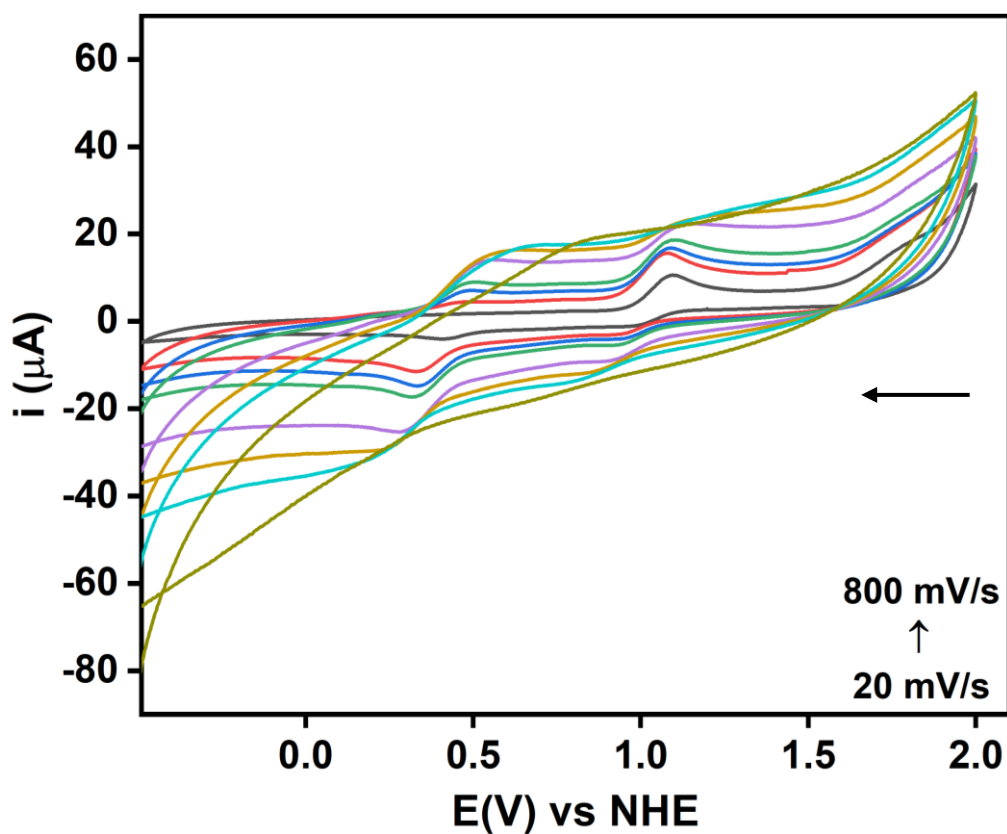


**Figure S42.** Plots of (a)  $i_{c1}/i_{c2}$  vs. inverse of the scan rate to obtain  $K^{III}_{O \rightarrow S}$  (b)  $\ln(i_{a2}/\sqrt{v})$  vs. inverse of the scan rate to obtain  $k^{II}_{O \rightarrow S}$  for S-O isomerization of DMSO ligand of complex **3a**.

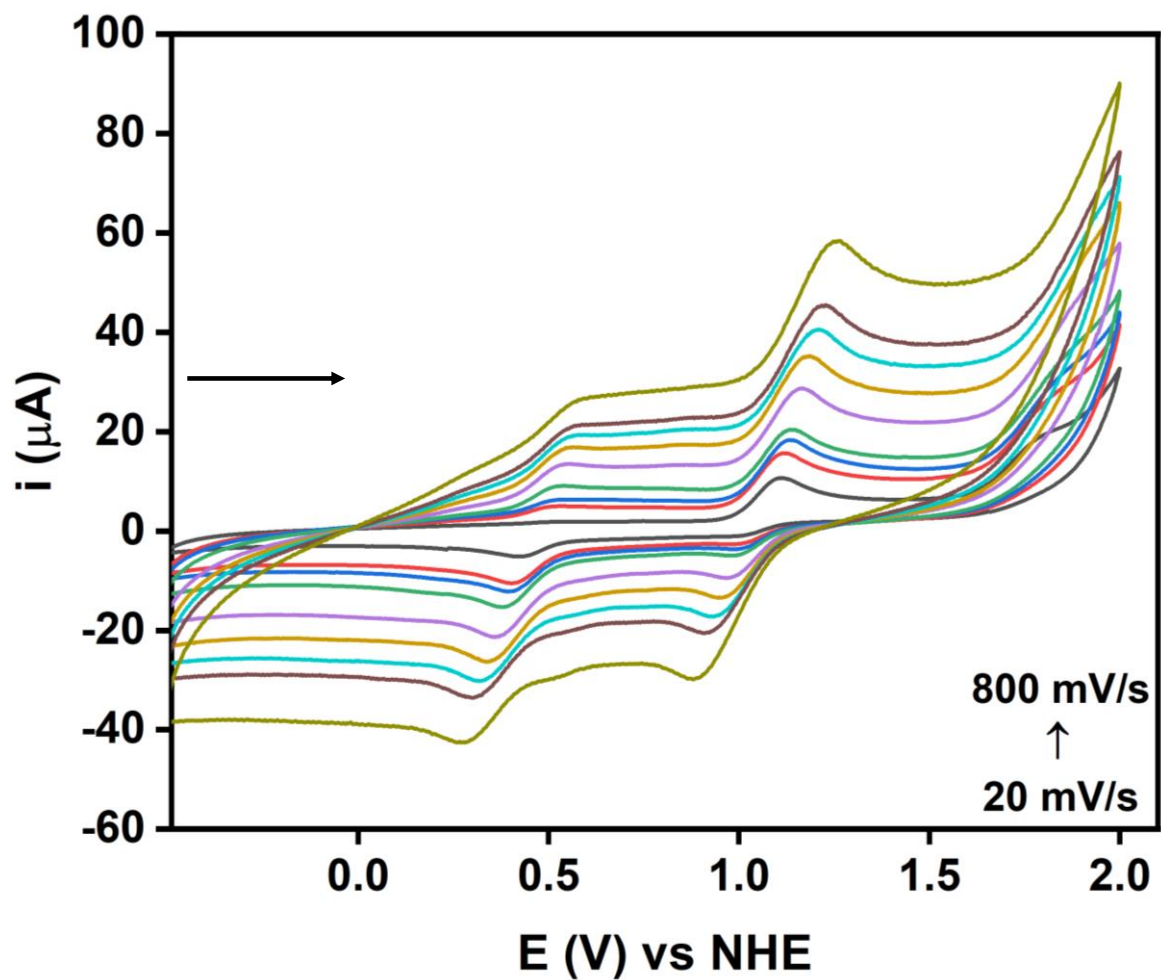


**Figure S43.** Plot of  $i_k/i_d$  vs.  $\sqrt{v}$  to obtain  $k_{O \rightarrow S}^{III}$  and  $k_{S \rightarrow O}^{III}$  for complex **3a**.

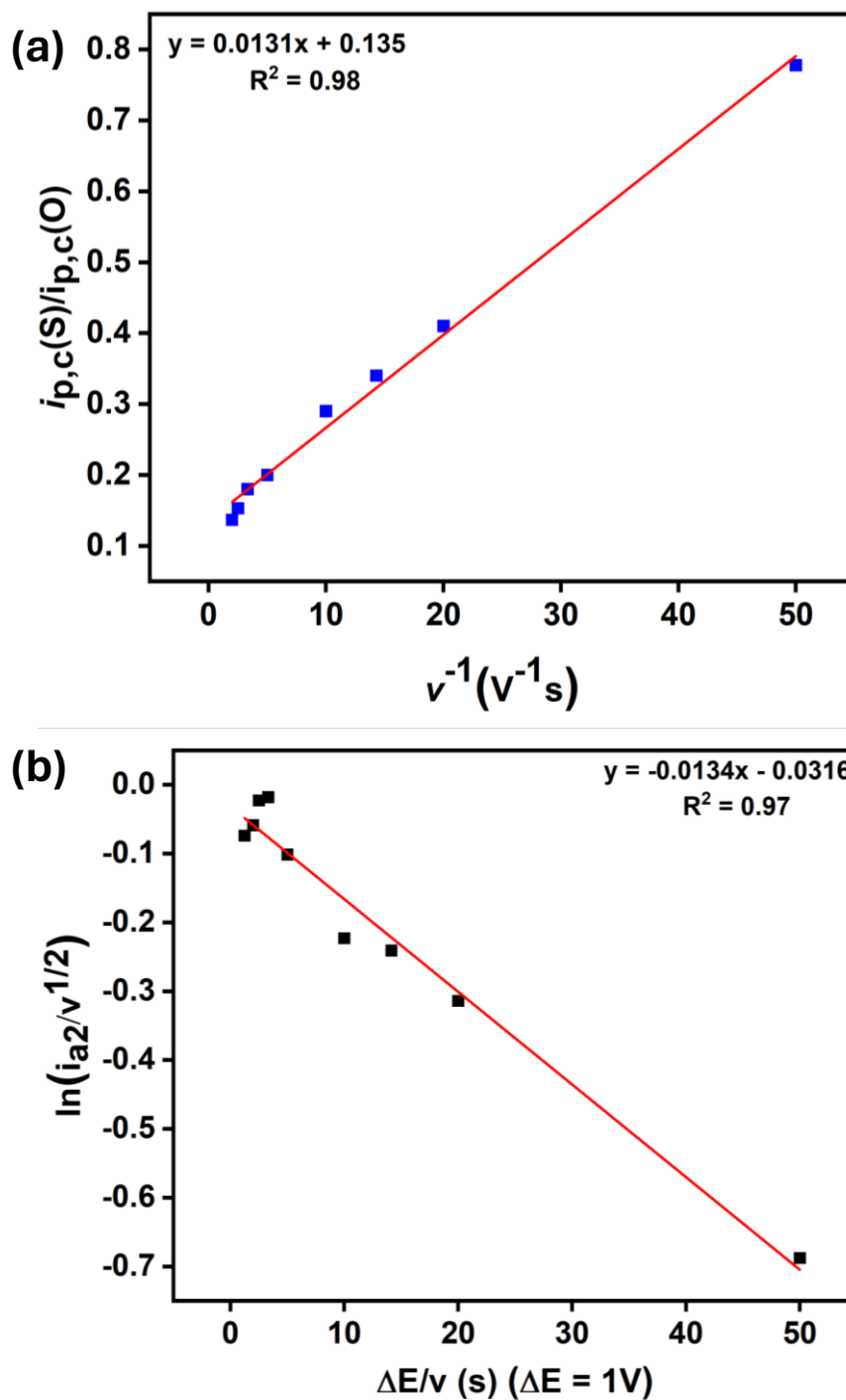




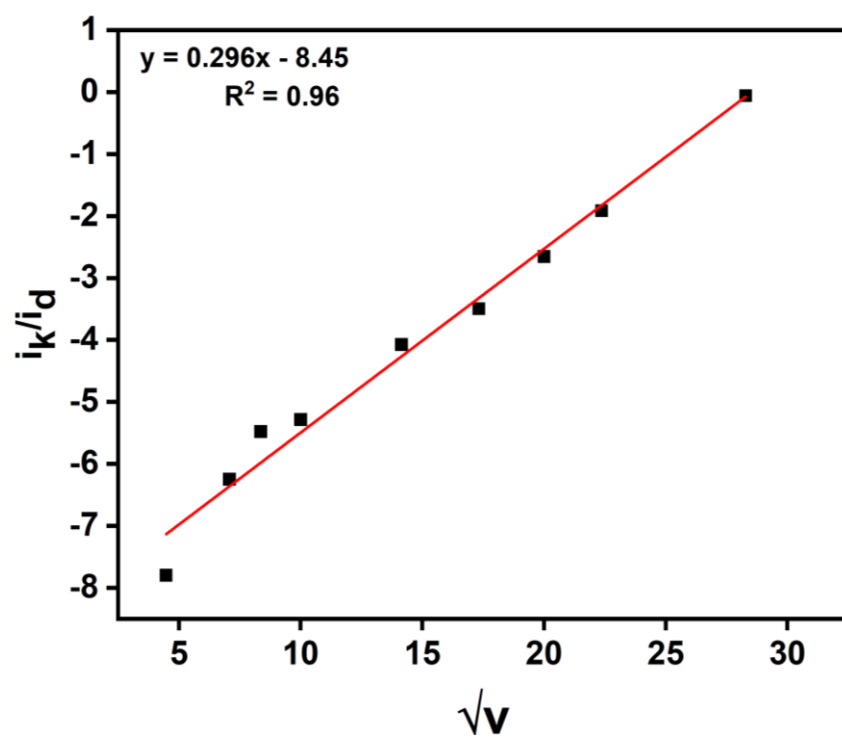
**Figure S44.** Cyclic voltammograms of **3b** in 0.1 M TBAH,  $\text{CH}_2\text{Cl}_2$ , at scan rates between 20 mV/s to 800 mV/s, after applying the CPE for 5 minutes at 2 V. Arrow indicates the starting potential and scanning direction.



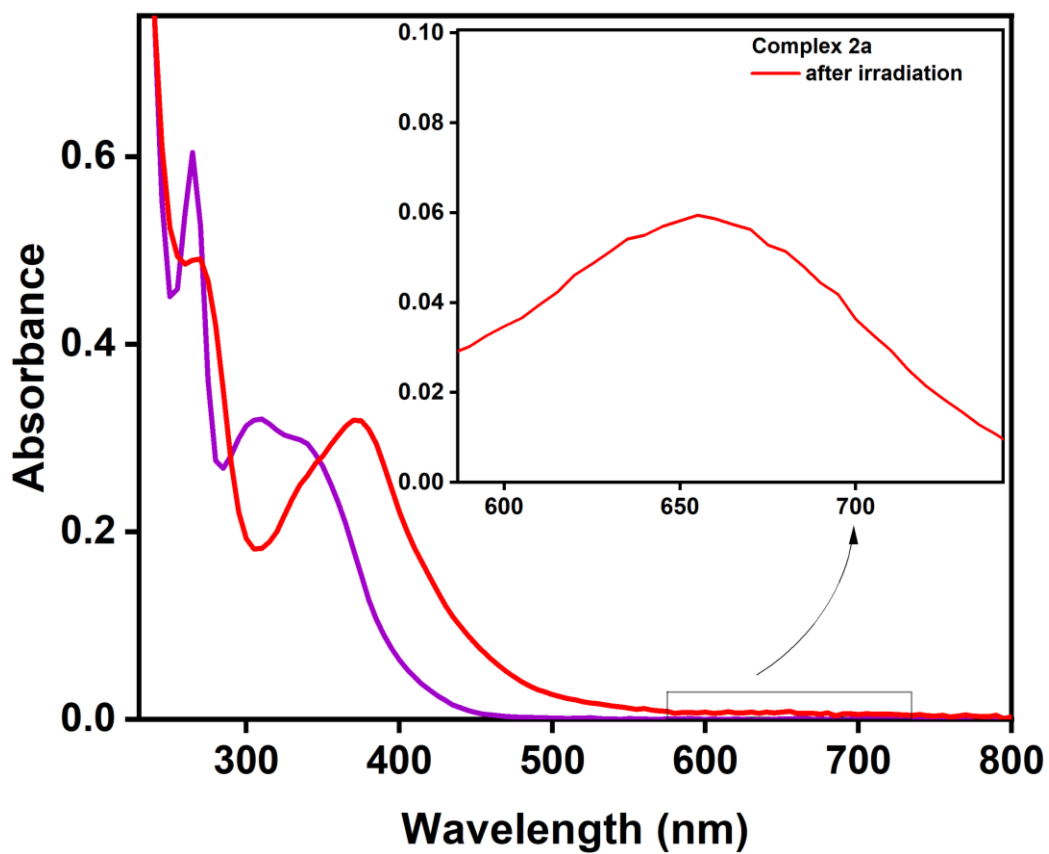
**Figure S45.** Cyclic voltammograms of **3b** in 0.1 M TBAH,  $\text{CH}_2\text{Cl}_2$ , at scan rates between 20 mV/s to 800 mV/s, after applying the CPE for 5 minutes at -0.5 V. Arrow indicates the starting potential and scanning direction.



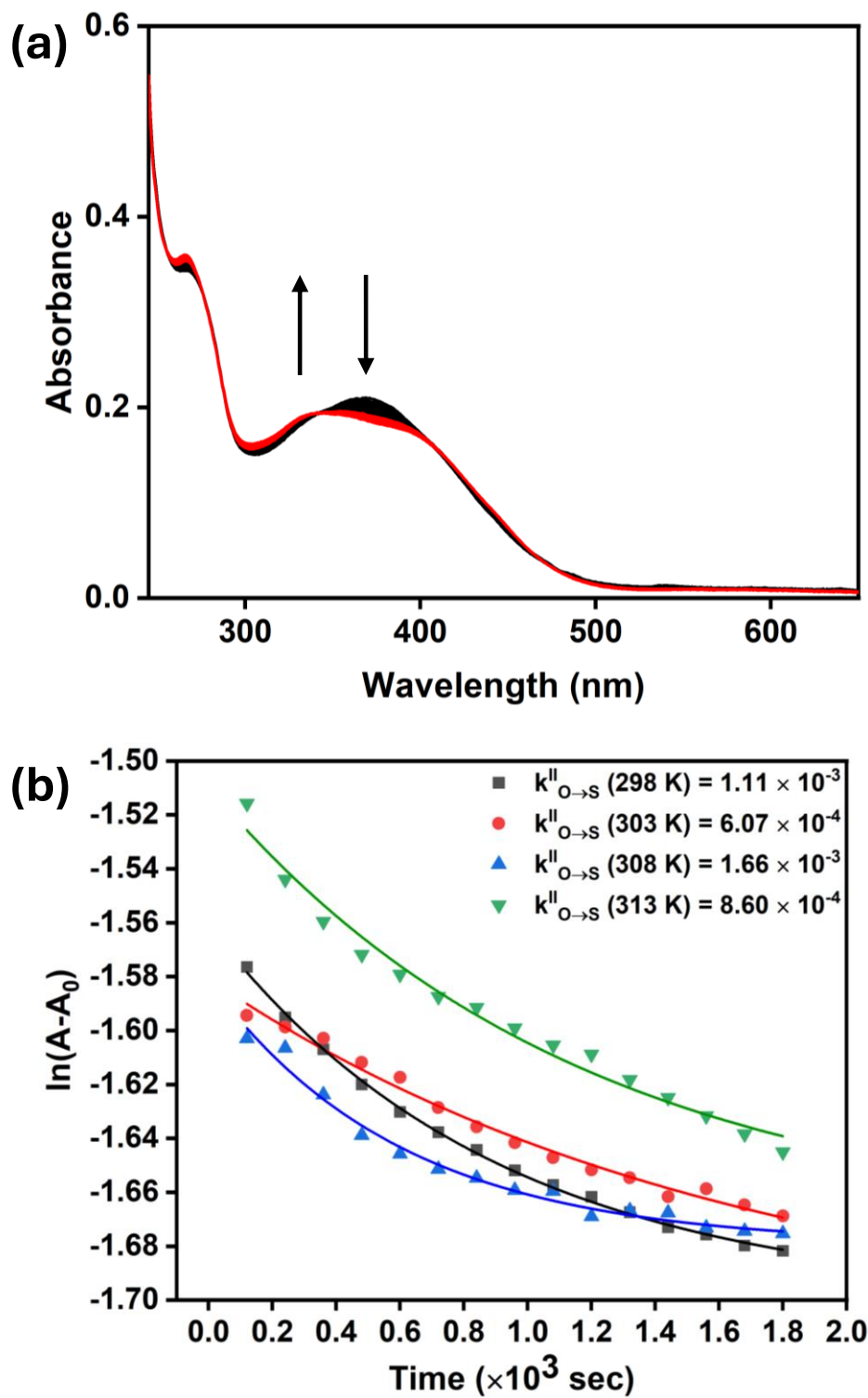
**Figure S46.** Plots of (a)  $i_{c1}/i_{c2}$  vs. inverse of the scan rate to obtain  $K^{\text{III}}_{\text{O-S}}$  (b)  $\ln(i_{a2}/\sqrt{v})$  vs. inverse of the scan rate to obtain  $K^{\text{II}}_{\text{O-S}}$  for S-O isomerization of DMSO ligand of complex **3b**.



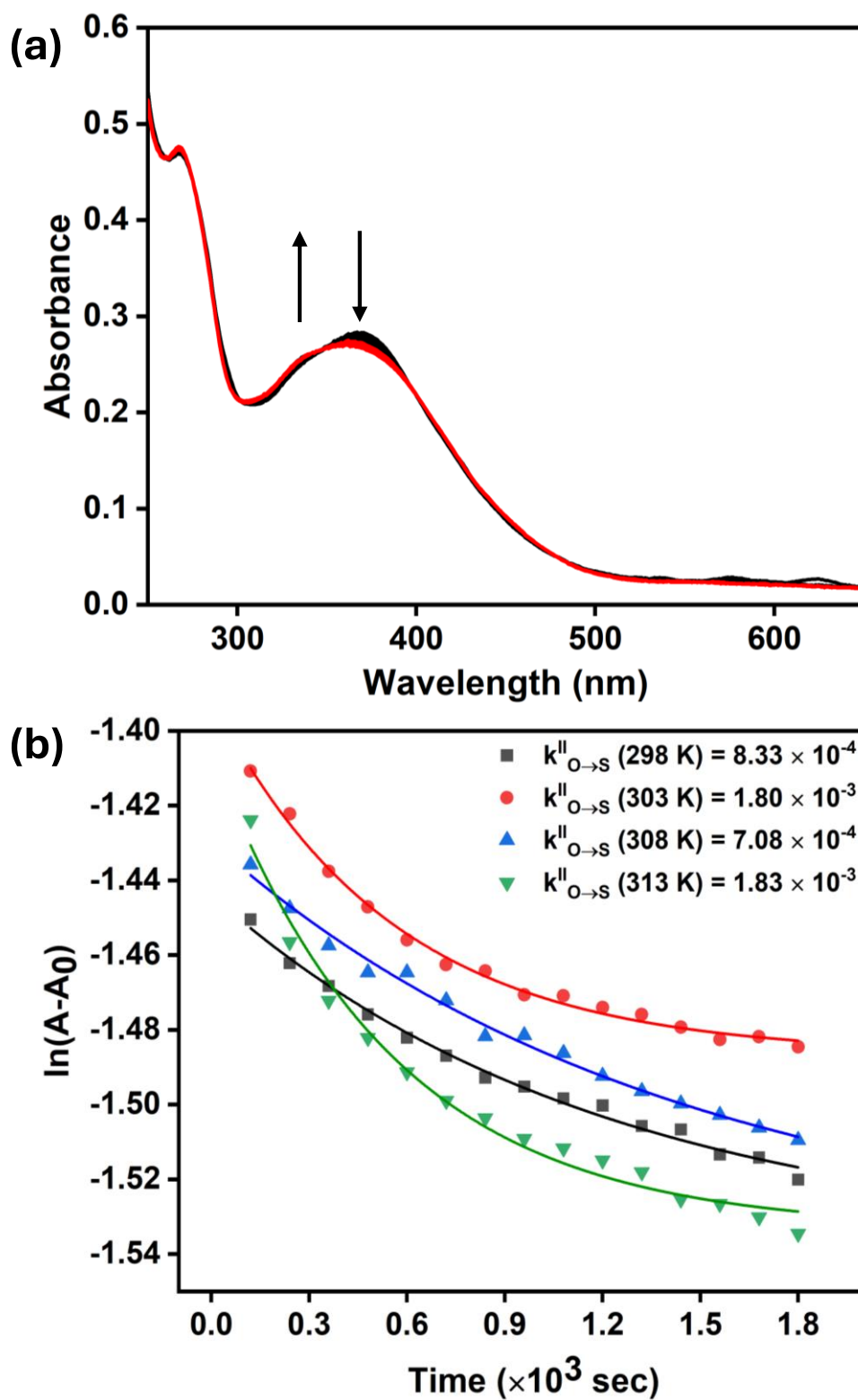
**Figure S47.** Plot of  $i_k/i_d$  vs.  $\sqrt{v}$  to obtain  $k^{\text{III}}_{\text{S} \rightarrow \text{O}}$  and  $k^{\text{III}}_{\text{O} \rightarrow \text{S}}$  for complex **3b**.



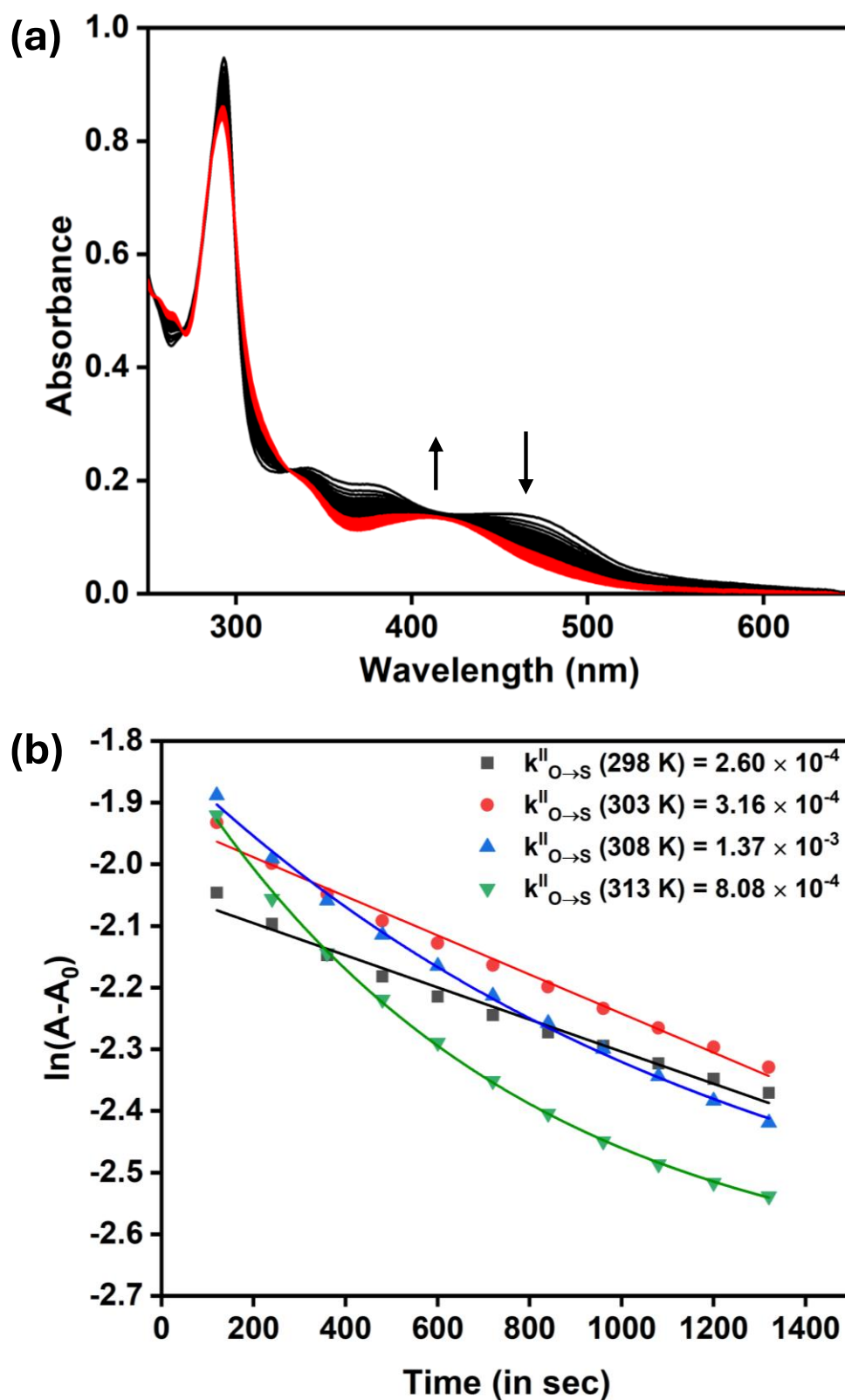
**Figure S48.** UV-vis spectrum of complex **2a** before and after irradiation, inset showing the lower energy absorption of irradiated sample of **2a**.



**Figure S49.** (a) UV-Vis spectra of O-bonded (black) and S-bonded (red) isomers of 2a in 10% DMSO in MeOH at 298 K and (b) kinetic data of 2a at 370 nm with exponential fit.

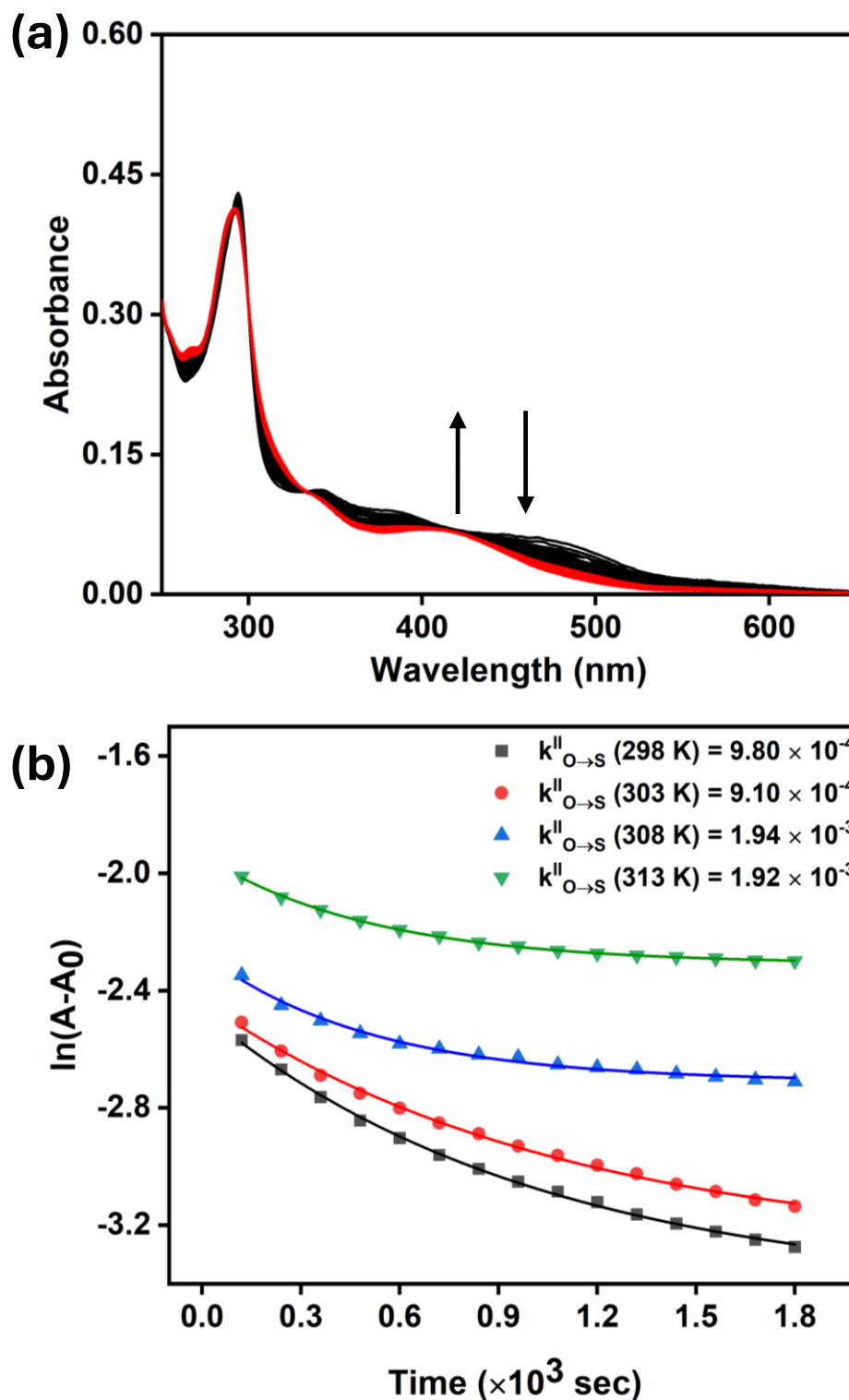


**Figure S50.** (a) UV-Vis spectra of O-bonded (black) and S-bonded (red) isomers of **2b** in 10% DMSO in MeOH at 298 K and (b) kinetic data of **2b** at 373 nm with exponential fit.



**Figure S51.** (a) UV-Vis spectra of O-bonded (black) and S-bonded (red) isomers of **3a** in 10% DMSO in MeOH at 298 K and (b) kinetic data of **3a** at 464 nm with exponential fit.

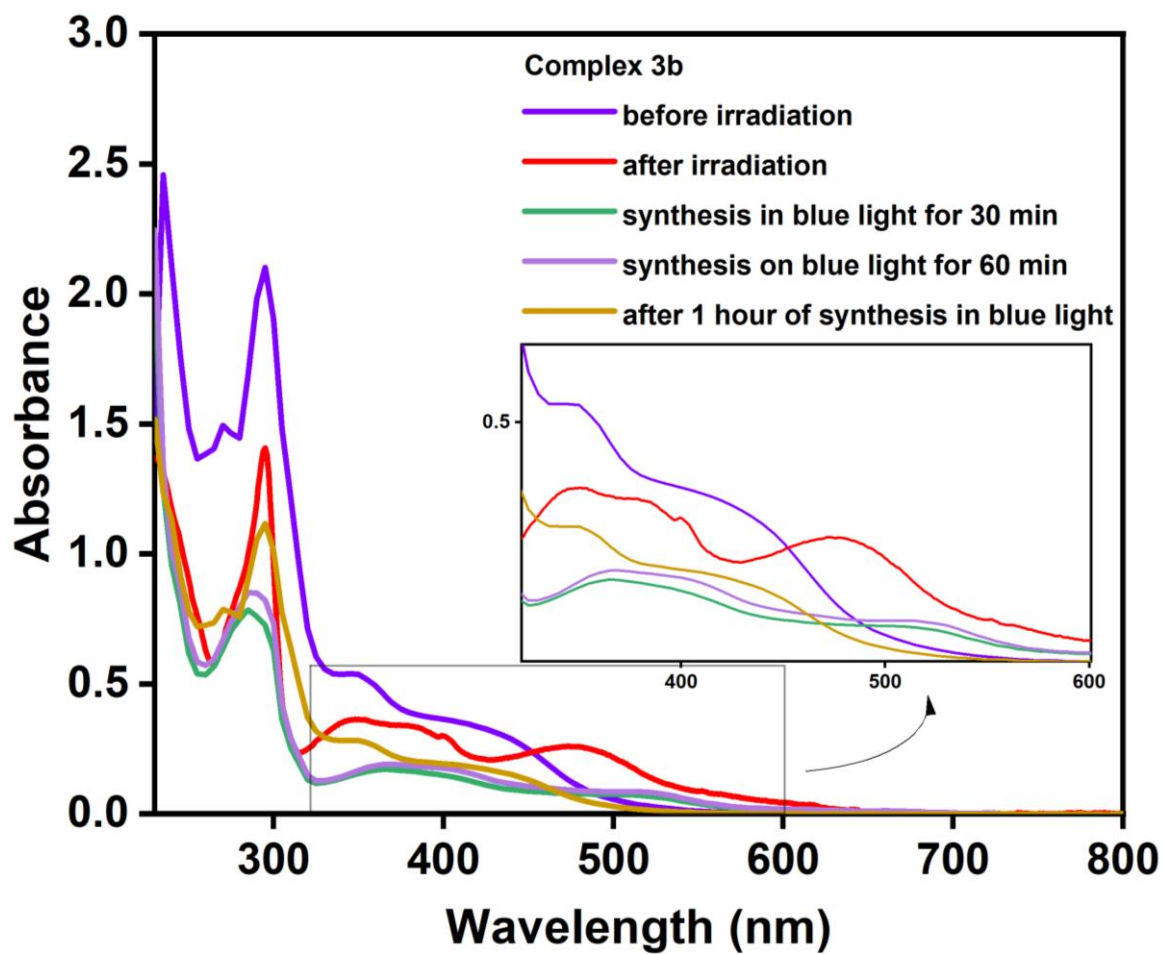




**Figure S52.** (a) UV-Vis spectra of O-bonded (black) and S-bonded (red) isomers of **3b** in 10% DMSO in MeOH at 298 K and (b) kinetic data of **3b** at 370 nm with exponential fit.

**Table S2. Reaction rates for the reversion of O→S isomerization in complexes 2a, 2b, 3a, and 3b at complex concentration of  $2.0 \times 10^{-3}$  mM in MeOH:DMSO (9:1).**

Complex	Temperature (K)	$k_{O \rightarrow S}^I$ ( $s^{-1}$ )	
		MeOH	MeOH:H <sub>2</sub> O (9:1)
<b>2a</b>	298	$8.19 \times 10^{-4}$	$9.2 \times 10^{-4}$
<b>2b</b>	303	$8.67 \times 10^{-5}$	$2.10 \times 10^{-5}$
<b>3a</b>	308	$4.82 \times 10^{-5}$	$4.76 \times 10^{-5}$
<b>3b</b>	313	$5.0 \times 10^{-5}$	$1.69 \times 10^{-5}$



**Figure S53.** Comparative UV-vis spectra of complex **3b** synthesized in thermochemical and photochemical reaction conditions.

**Table S3.** Crystallographic parameters for complex **2a**.

	<b>2a</b>
<b>Empirical formula</b>	C <sub>13</sub> H <sub>21</sub> Cl <sub>2</sub> N <sub>3</sub> O <sub>2</sub> RuS <sub>2</sub>
<b>Fw/g M<sup>-1</sup></b>	487.433
<b>Crystal system</b>	monoclinic
<b>Space group</b>	<i>P2<sub>1</sub>/n</i>
<b><i>a</i>/Å</b>	9.1097(2)
<b><i>b</i>/Å</b>	14.8835(3)
<b><i>c</i>/Å</b>	13.8216(3)
<b><i>α</i>/°</b>	90
<b><i>β</i>/°</b>	94.137(2)
<b><i>γ</i>/°</b>	90
<b><i>V</i>/ Å<sup>3</sup></b>	1869.11(7)
<b><i>Z</i></b>	4
<b><i>T</i>, K</b>	293(2)
<b><math>\rho_{\text{calcd}}</math>/Mg m<sup>-3</sup></b>	1.732
<b><math>\lambda</math>/Å (Mo/Cu-K<math>\alpha</math>)</b>	0.7107
<b>Data/restr./param.</b>	3997/0/213
<b><i>F</i>(000)</b>	981.618
<b>GOOF</b>	1.2555
<b>R (int)</b>	0.1306
<b><i>R</i>(<i>F</i><sub>o</sub>),<sup>a</sup> <i>I</i> &gt; 2 <math>\sigma</math>(<i>I</i>) [<i>wR</i>(<i>F</i><sub>o</sub>)<sup>b</sup>]</b>	0.0588 [0.1234]
<b><i>R</i> (all data) [<i>wR</i> (all data)]</b>	0.0966 [0.1735]

**Table S4.** Selected bond lengths and angles for the complex **2a**.

Complex	Bond lengths (Å)		Bond Angles (°)	
<b>2a</b>	Ru1-C1	1.992(6)	C1 Ru1 N1	78.6(2)
	Ru1-N1	2.077(5)	C1 Ru1 Cl1	100.10(17)
	Ru1-Cl1	2.4347(16)	C1 Ru1 Cl2	171.49(16)
	Ru1-Cl2	2.4770(17)	C1 Ru1 S1	88.50(6)
	Ru1-S1	2.3026(18)	C1 Ru1 S2	93.24(6)
	Ru1-S2	2.3021(18)	N1 Ru1 Cl1	178.12(14)
			N1 Ru1 Cl2	93.52(15)
			N1 Ru1 S1	90.13(14)
			N1 Ru1 S2	88.06(14)
			Cl1 Ru1 Cl2	87.81(6)
			Cl1 Ru1 S1	88.50(6)
			Cl1 Ru1 S2	93.24(6)
			Cl2 Ru1 S1	92.19(6)
			Cl2 Ru1 S2	90.92(6)
			S1 Ru1 S2	176.49(6)

## XYZ Coordinates

### 2a: [Ru(CN)(Cl)<sub>2</sub>(S-DMSO)<sub>2</sub>]

Ru	1.24352286250027	-0.06062185735257	-0.03982825649056
S	1.43182881148262	-1.46939524891577	-1.87095052827295
S	1.06256351444319	1.35521755287920	1.78109865924453
Cl	3.22331759589192	1.10206926166530	-0.88335979818922
Cl	2.77850036228090	-1.49379855672693	1.30581320655012
N	-0.44288806469017	-1.14001450706831	0.52455908536258
N	-1.46897226347506	0.44497590338835	-0.76314195029373
O	0.35311909511957	-2.50501512667299	-2.06498924002171
O	-0.06706865144725	2.35788378648874	1.77190059425117
C	-0.18903793752346	0.97133529055174	-0.91736301058250
C	-1.60820261268140	-0.71832835743796	-0.01820745243940
N	-0.40714375913373	2.13905773871096	-1.57445551627224
C	-0.45489104119097	-2.27967647549208	1.24210504976978
H	0.51366797991608	-2.58738767780688	1.62719016617548
C	-2.43673631898512	1.28774810883137	-1.29563370920453
H	-3.49241634598825	1.07314502081562	-1.27947413191741
C	-2.81182493585153	-1.38626681150477	0.15787489776272
H	-3.72118727951778	-1.01358863979298	-0.29870572606602
C	-1.76583816003623	2.34659314387145	-1.79552374450544
H	-2.13340089962863	3.23057691351920	-2.29338910381401
C	-1.61491634450806	-3.00063202417570	1.46148737672796
H	-1.57064429558506	-3.91244064781548	2.04611093667570
C	-2.81215441705615	-2.54641868473059	0.91594982585583
H	-3.73633045884187	-3.09386662946004	1.06958682217870
C	1.53854253601182	-0.51820504689374	-3.42588213124641
H	0.57796909318247	-0.01084131139658	-3.54167435457203
H	2.35125419691844	0.20712246907403	-3.33507332437926
H	1.69955267336174	-1.22653738972319	-4.24288753927939
C	3.04622046873898	-2.30866871684207	-1.93400906455425
H	3.82536093191721	-1.55456784522672	-1.79409898815719
H	3.05847084818764	-3.01265724542164	-1.10079586227053
H	3.11708459930231	-2.81896689315456	-2.89836756182689
C	0.60089767570428	3.16746818389964	-1.80324199391027
H	1.58889123461135	2.71499161464818	-1.69908074607566
H	0.48223303245686	3.58071197072573	-2.80958232628744
H	0.48429796390128	3.96380493445839	-1.05989749187827
C	0.91701961812683	0.43244992383955	3.35263259614872
H	0.04571405927787	-0.21974044493142	3.26100624400089
H	1.82001734420968	-0.16244814050139	3.50239295745991
H	0.75765438896850	1.17271384294377	4.14160061816993
C	2.61791006872968	2.23193681188174	2.14095903933193
H	3.41149288224084	1.48332858226060	2.21706145889170
H	2.81915542266007	2.89163603299002	1.29629658264980
H	2.47339452599829	2.79031719160081	3.06998743529985

### 2a<sup>+</sup>: [Ru(CN)(Cl)<sub>2</sub>(S-DMSO)<sub>2</sub>]<sup>+</sup>

Ru	1.34041350958115	-0.00601011236856	-0.05150535029626
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S	1.43743431446549	-1.49546706150252	-1.88614952366364
S	1.24391589174319	1.51846103121414	1.73928813356562
Cl	3.09259906161255	1.20019258405305	-0.99485118576072
Cl	2.73961126939564	-1.39732206199448	1.28248835761877
N	-0.38129091338248	-1.14579591025129	0.54214703779344
N	-1.45436645891942	0.42407896432465	-0.73610765219329
O	0.32292184313593	-2.49643128193423	-1.96382996982435
O	0.44623231998523	2.76465545174057	1.48805204365424
C	-0.22520734879385	1.02293229044795	-0.86990758129036
C	-1.54826306609193	-0.76658731429840	-0.01573777613375
N	-0.48092378454528	2.20247548825101	-1.46516453769200
C	-0.36271283911325	-2.29630281671125	1.24414019564943
H	0.59717774001893	-2.58512456726189	1.65604981837418
C	-2.46258258881357	1.23005630200855	-1.25159560914396
H	-3.50661240600693	0.96423679008105	-1.23776141786092
C	-2.72509224681133	-1.48748235998258	0.11248345902444
H	-3.63644214768196	-1.15022822041936	-0.36651628301187
C	-1.84386108784635	2.33687825155964	-1.71245044643630
H	-2.24928039881556	3.21795769027619	-2.18630371543382
C	-1.49636013064408	-3.06564139727951	1.42621049102374
H	-1.42749828856651	-3.97897378119028	2.00596756451343
C	-2.69468454569128	-2.65961179380899	0.85010869313874
H	-3.59608437135866	-3.25263207571758	0.96530989505300
C	1.48554178537160	-0.59170932545943	-3.46803058432076
H	0.54572902740694	-0.03966050682240	-3.54525395511582
H	2.33860826389052	0.09029508799320	-3.47218073007991
H	1.55286630466271	-1.33898987738302	-4.26335452393548
C	3.03655999698745	-2.35662258759398	-1.96847108705643
H	3.83423619457982	-1.60908150513129	-1.94178134458026
H	3.09425136168259	-3.00232095478978	-1.09060009329396
H	3.04667118271240	-2.94009043049457	-2.89309064847809
C	0.46316849282025	3.28576590776174	-1.74531314992105
H	1.43660970698727	3.03026712113250	-1.33602754038851
H	0.54185143607075	3.43763453572408	-2.82605607085464
H	0.09914806775122	4.19646469517908	-1.26341603461238
C	0.59766595688112	0.71161872438511	3.23946665077399
H	-0.43202835151075	0.41582910738779	3.02583868642727
H	1.21605422387596	-0.16100310586993	3.46653745506367
H	0.62129480450639	1.44889001414167	4.04649298184097
C	2.89986294729522	1.98752346300231	2.32742516892107
H	3.46794525466975	1.07880344973375	2.54157247925926
H	3.37164834321737	2.55341583505973	1.52243514930469
H	2.75927167328572	2.60965626280755	3.21544255037861

**2a': [Ru(CN)(Cl)2(S-DMSO)(O-DMSO)]**

Ru	1.32019574607936	-0.27155428711160	-0.13992963339719
S	1.40589928301946	-1.44129257340053	-2.02625500246209
Cl	3.33469202359107	0.97752304151199	-0.72873702608382
Cl	2.78331058533352	-1.85646961351035	1.14325630568235
N	-0.39651064017579	-1.26245856270663	0.44852647400970

N	-1.37132903957064	0.48515304378909	-0.65023156096026
O	0.26663135832056	-2.36430267159132	-2.37720454904776
C	-0.05827525072063	0.90760095797974	-0.87404183187712
C	-1.56050476899064	-0.69570988232010	0.05539812566851
N	-0.22872350460347	2.09113740589658	-1.53174573149756
C	-0.46130478168010	-2.41780174412834	1.13657137874133
H	0.50086016263780	-2.83370469338331	1.42075751476891
C	-2.29835641221791	1.38050672947028	-1.16526961429861
H	-3.36512535764107	1.24272011646043	-1.10089456986190
C	-2.80565771751552	-1.24489401503975	0.32716391149871
H	-3.71132663787483	-0.75903727539718	-0.01704413934294
C	-1.57782368252066	2.38098980250761	-1.71577690551049
H	-1.90485872829154	3.27697191567083	-2.22093814954840
C	-1.66454805952037	-3.02569043158760	1.44896656510286
H	-1.65920551005081	-3.95892156988966	2.00096127982357
C	-2.85548606849318	-2.43404794452617	1.03842253683523
H	-3.81273836904737	-2.89358636203675	1.26254640372711
C	1.64030822605869	-0.35825592287680	-3.48508365561577
H	0.71606219316568	0.21505852853040	-3.58908018509328
H	2.49085828159220	0.30184157874529	-3.29452176803129
H	1.79155285087369	-0.99393705501887	-4.36168662214165
C	2.95981329400029	-2.38892188770504	-2.15067273870133
H	3.78994169996308	-1.70176935045644	-1.96438096408124
H	2.92608713975366	-3.14360982922803	-1.36392767398429
H	2.99611596505307	-2.84030627108121	-3.14599569957266
C	0.84177430149141	2.96236107573548	-1.99814147956023
H	1.79397575966007	2.55589323898194	-1.64946504133095
H	0.83959317222327	3.01066743072776	-3.09336861552912
H	0.69880141240980	3.97021372396438	-1.59440443587724
O	1.24500383057720	0.85316349496014	1.70979667986416
S	2.61258900511554	0.94669999375087	2.46514286957463
C	2.58055735051784	2.68294291439454	3.03594536532123
H	1.61018000017461	2.90056035626533	3.49066300414576
H	3.39724807060788	2.84277645017657	3.74668874165409
H	2.73438842745598	3.29785891175927	2.14599796260260
C	2.25267068125954	0.15972080763615	4.07361552680499
H	2.17704355272107	-0.90966742284091	3.86447720692001
H	3.08231058203516	0.35574488443655	4.76017072032314
H	1.31030957322298	0.55453296248537	4.46382902033831

**2a<sup>+</sup>: [Ru(CN)(Cl)<sub>2</sub>(S-DMSO)(O-DMSO)]<sup>+</sup>**

Ru	1.42228131861352	-0.28515629943943	-0.15918405235379
S	1.45032309067447	-1.55321432011436	-2.03828034955878
Cl	3.21137871301803	1.00589394759604	-0.86136745366347
Cl	2.72766429119895	-1.84726558349540	1.07088930162317
N	-0.37315470711549	-1.28589383647274	0.42769704304925
N	-1.32903727728713	0.53598096048117	-0.57401532177081
O	0.31666968743223	-2.51695812843870	-2.21054940458937
C	-0.04656215534337	0.93792224851274	-0.84784635933927
C	-1.52471767971533	-0.67943654077650	0.08537390675009



N	-0.18727860282375	2.13999464475265	-1.44852661934125
C	-0.44712276452128	-2.48814154563740	1.02816450113441
H	0.49949852709582	-2.95673426582081	1.26959924023437
C	-2.25639286626301	1.47690866605955	-1.00339653889160
H	-3.32141701434482	1.36493701548306	-0.88652781523435
C	-2.77676523593810	-1.21574595615103	0.34065587712097
H	-3.67735842102147	-0.69301553180966	0.04163396050758
C	-1.53465085387713	2.47721928670076	-1.55135370188095
H	-1.85732567124347	3.40109608696853	-2.00575752551420
C	-1.65742181549706	-3.09067168479227	1.31957069723803
H	-1.66236195416884	-4.05965450719185	1.80532303242182
C	-2.83967637891122	-2.44699159634404	0.97401723667831
H	-3.80253257205013	-2.90054896897942	1.18507349153206
C	1.52544389985148	-0.52151986401629	-3.54089184786705
H	0.60267704054559	0.06304264986332	-3.57008702540307
H	2.40297851103475	0.12766541143797	-3.48595498714116
H	1.57121489069055	-1.19666008872800	-4.39959634979383
C	3.02461272592312	-2.44908530587920	-2.21698144879845
H	3.84636913164870	-1.73562401993239	-2.11028214805694
H	3.05970681775082	-3.18873482969941	-1.41597185652465
H	3.01611164948180	-2.92835847586897	-3.19956632322528
C	0.88827289584745	3.01855722883455	-1.91284983989728
H	1.52010250574017	3.31530446096572	-1.07392648728655
H	1.50698990697730	2.50699585493284	-2.65207159863917
H	0.43312970494684	3.90088086403022	-2.36559309659028
O	1.30301833035148	0.88898275780528	1.64744078516458
S	2.62273341448444	1.02048958405951	2.49670046678046
C	2.53996564807516	2.75365523247521	3.04512743977482
H	1.54419860385884	2.95927515898063	3.44683497196174
H	3.31342859490297	2.91886983234654	3.80126829571085
H	2.74085028449954	3.37346357524243	2.16848289366544
C	2.19770450095452	0.22213875983539	4.07705581329792
H	2.14942667341236	-0.85010094189143	3.87620428894930
H	2.99116618968548	0.43453274295218	4.80022614512966
H	1.23285842142521	0.60240532116299	4.42333876263671

**2a'': [Ru(CN)(Cl)<sub>2</sub>(O-DMSO)<sub>2</sub>]**

Ru	1.34633837719755	-0.13812621841017	0.05138526454529
Cl	3.34972961875578	1.14286933317280	-0.54781895998837
Cl	2.85867452955019	-1.80199293709388	1.27290278625666
N	-0.31952342335320	-1.19449265978887	0.53024965624150
N	-1.30989822060570	0.47569812036927	-0.66250921056207
C	0.00696284456652	0.95263398033073	-0.79310946427968
C	-1.49477485499377	-0.69037114849739	0.05698132366468
N	-0.16834571781537	2.10025022075510	-1.52468013959744
C	-0.38963086572268	-2.33560095615471	1.25491865575117
H	0.56668172090959	-2.70353950425168	1.61359752991993
C	-2.22980596336879	1.30386987378720	-1.29157679383833
H	-3.29135008581920	1.11836006423001	-1.30791073969712
C	-2.72821221129630	-1.28478494394330	0.27860409268251

H	-3.63098251212448	-0.83902064475248	-0.12429488667708
C	-1.50945975575906	2.31239608450205	-1.82697303021666
H	-1.83379456515849	3.16845427027852	-2.39917601946821
C	-1.58458110515163	-2.98221253791193	1.51629205796152
H	-1.57200826073412	-3.89399666938450	2.10401605464677
C	-2.77681424447407	-2.45592516199798	1.02370365935948
H	-3.72692310090235	-2.94419605940688	1.21395246431658
C	0.88552251336939	3.00507134877035	-1.95789339737291
H	1.83510510727680	2.64621381694368	-1.55646455108287
H	0.93767527848961	3.02637952482832	-3.05279660165900
H	0.68288897276673	4.01680302456871	-1.58822069210099
O	1.21138375380075	0.94854025229266	1.86454254710248
S	2.58765355628117	1.05012068105236	2.61127223673184
C	2.54610629648514	2.78416879990088	3.18522356824133
H	1.57391405730496	2.99332153498400	3.63997094178916
H	3.36204163664841	2.94766547743322	3.89598080904446
H	2.69528395083279	3.39960522215473	2.29487147896744
C	2.23139795338981	0.24960935659491	4.21450680099277
H	2.16036859498058	-0.81841582172423	3.99563923189098
H	3.06170925684449	0.44205045739597	4.90136149568455
H	1.28781291680036	0.63664304560055	4.60919075067277
O	1.60388181989648	-1.31178976123764	-1.69107804206667
S	3.08263182968293	-1.80324156192823	-1.87684305701102
C	3.31399099243754	-1.54822608939469	-3.67106477483442
H	3.39537733720176	-0.46798525646698	-3.81312719914272
H	4.23856851854811	-2.04041866854679	-3.98821251590457
H	2.44794124359716	-1.94406625572246	-4.20867254658082
C	2.89177253575163	-3.61962217325870	-1.90524457322541
H	3.83385166136784	-4.07329716336865	-2.22914195180338
H	2.67014665983558	-3.90324072626057	-0.87364365655520
H	2.06869135270952	-3.88516157044327	-2.57441060279893

**2a<sup>++</sup>: [Ru(CN)(Cl)<sub>2</sub>(O-DMSO)<sub>2</sub>]<sup>+</sup>**

Ru	1.49039267418226	-0.10959854933315	0.05223683571934
Cl	3.40848748898351	1.14398056095230	-0.53552874046006
Cl	2.97471107322149	-1.71138795077171	1.22887080000667
N	-0.23759123001562	-1.19097259376049	0.53490251446788
N	-1.21357875180064	0.49316514302688	-0.66170255487420
C	0.07485024137143	0.99193585704702	-0.80556644894115
C	-1.39340931043188	-0.67932494599113	0.05920210407694
N	-0.09849756602748	2.12450990302632	-1.52582000963499
C	-0.28629125473726	-2.32786391990268	1.25586982733735
H	0.67364494781730	-2.69113507620435	1.61158059242804
C	-2.14774861637040	1.30867746281403	-1.28627692028200
H	-3.20696601187511	1.11077796465801	-1.29716966144222
C	-2.62920202700572	-1.27467971965856	0.27883830928997
H	-3.53702117122635	-0.83660093330690	-0.11890364299555
C	-1.44182559433075	2.32541276748539	-1.82521865790193
H	-1.77605431046786	3.17878612539713	-2.39570372526524
C	-1.47800428521181	-2.97758418428805	1.51756045026227

H	-1.47172319824100	-3.89012843202011	2.10277956804551
C	-2.66540843600094	-2.44343323123928	1.02136100103802
H	-3.61471599832224	-2.93370957495073	1.21171922224505
C	0.94640763332673	3.04614693629236	-1.97055569285913
H	1.89663219219551	2.73695801731627	-1.53683498400902
H	1.01669367131449	3.02279479209606	-3.06249382319508
H	0.69523026782455	4.05967507436098	-1.64482008976590
O	1.26545756305191	0.93352262640551	1.79655792971097
S	2.59641447460156	1.09643199867827	2.67394969634893
C	2.37392129229762	2.80150519035149	3.26067917821758
H	1.35932324634460	2.92620366924996	3.64747429129312
H	3.12171120804196	2.99991973052356	4.03452357806670
H	2.54733466574759	3.45265664694415	2.40082130093632
C	2.15504288089240	0.20809967868504	4.19624582065643
H	2.17679922217582	-0.85409760681791	3.94292367049030
H	2.91359026085680	0.43015218879235	4.95333434253763
H	1.16114064539655	0.52331857109514	4.52430699964223
O	1.64529677900585	-1.24512232232126	-1.64296090990673
S	3.10423831426295	-1.83205832614304	-1.94718322086279
C	3.14888816055432	-1.63334379455928	-3.75274628994427
H	3.25802837893476	-0.56373531254046	-3.94621951246183
H	4.02023065866566	-2.17213871803752	-4.13717117885394
H	2.22167280367751	-2.01683608648967	-4.18613100657190
C	2.81410301826769	-3.62383652522180	-1.86185254312972
H	3.69343424149355	-4.13258179481787	-2.26903306888873
H	2.69924479044252	-3.86250965569866	-0.80220604692426
H	1.91311496711611	-3.87095165112360	-2.42933930364662

**3a<sup>+</sup>: [Ru(CN)(bpy)(Cl)(S-DMSO)]<sup>+</sup>**

Ru	1.04556150563445	-0.22395465303309	0.22903153456426
S	0.72475533066874	1.25602882900285	1.95598380787824
Cl	2.88692552959639	1.05928433165706	-0.65905409740132
N	-0.54100416526451	-1.38280846060488	0.89124765245483
N	-1.692404444056655	-0.06790086453533	-0.58687735483057
O	1.18972685637958	0.85707664683927	3.33538799160702
C	-0.47378652921616	0.58237135986024	-0.77524351304526
C	-1.74109206331190	-1.12891913654385	0.31504108901044
N	-0.77547608292621	1.55525091115818	-1.67222873181864
C	-0.47821371075044	-2.36956553473488	1.80855048118683
H	0.49589109358337	-2.53098474176480	2.25814888740808
C	-2.70374050339813	0.50401331965894	-1.35174918136583
H	-3.72424418788567	0.15691008646166	-1.35691473420830
C	-2.89239348832228	-1.84156109669233	0.61798077401843
H	-3.83346114144965	-1.60841452191220	0.13309069535085
C	-2.12209627809772	1.51694415125023	-2.02901296509944
H	-2.54545533303057	2.21561226802103	-2.73496251127878
C	-1.58169510884788	-3.12203237975847	2.16516403516892
H	-1.47800433500080	-3.90192437535476	2.91100246873761
C	-2.80722616812141	-2.85745700266403	1.55909133558692
H	-3.68996457178151	-3.43234061558306	1.81836521736502

C	0.16807365345812	2.52482465121478	-2.22982347358140
H	1.15618511528796	2.33208612026668	-1.80701468191320
H	0.21191776760761	2.41170324773656	-3.31741961975772
H	-0.16193741096478	3.54054209338582	-1.98925579926704
C	1.38843412886254	2.92432982717812	1.63848639388555
H	2.46695433104886	2.81540810067031	1.51472182765707
H	0.95432674871843	3.32074002827161	0.71741138468731
H	1.14083556742364	3.53950644396899	2.50777429410679
C	-1.03754991598564	1.70434830058550	2.16870640448143
H	-1.42659028320762	2.16669942001299	1.25751824660927
H	-1.58188371397209	0.78653074041074	2.40277638351714
H	-1.08932832776216	2.39211876732255	3.01667108976276
N	2.60102911216518	-1.41658703732350	1.11553992282899
C	3.14107040293410	-1.24836833783331	2.33455249712718
C	3.15248545231996	-2.33552183884671	0.28210608819247
C	4.23774218981889	-1.97542019424686	2.77274147307365
H	2.66430559675001	-0.50308444908292	2.96539215655031
C	4.25683754482654	-3.09383027062357	0.66648026353845
C	4.80987219159815	-2.91242171785927	1.92392548456928
H	4.63351844569407	-1.79177450858937	3.76576415161184
H	4.69363567255788	-3.81591665526657	-0.01230017282601
H	5.67503831075856	-3.49120157221594	2.23095382365422
C	2.50707250079490	-2.47207038987759	-1.02721124696464
C	2.90782210148161	-3.40065518667338	-1.98866634838509
N	1.46425406930054	-1.63616663225931	-1.26095199913757
C	2.24266114066849	-3.47245975937348	-3.20027166146894
H	3.74059299005616	-4.06455650343712	-1.79349002699604
C	0.82395262602186	-1.71150577025546	-2.44040202932375
C	1.17718283478879	-2.61019938100451	-3.43035009513589
H	2.55245359917417	-4.18879560656164	-3.95413600411245
H	0.00698165151715	-1.01416531480509	-2.58938880323647
H	0.62685169836696	-2.62336513561681	-4.36468280503679

**3a<sup>2+</sup>: [Ru(CN)(bpy)(Cl)(S-DMSO)]<sup>2+</sup>**

Ru	1.00185164082939	-0.19449764021723	0.13605259491784
S	0.62723050819801	1.24286287771574	1.93965175803701
Cl	2.55026920940836	1.19122320036143	-0.83329439591370
N	-0.55367568963799	-1.44548811840345	0.87872965952053
N	-1.81844456375925	-0.18872146227288	-0.56341394989900
O	0.47348671132696	0.47777402221520	3.22436273381962
C	-0.66284902032959	0.50501715588393	-0.81929539630203
C	-1.78581922313151	-1.23099455804794	0.37243966670044
N	-1.01534631796382	1.44643817130967	-1.71821409734884
C	-0.41023368901199	-2.39305675675912	1.82570249724052
H	0.58470763372467	-2.52482072263084	2.23279965012865
C	-2.88360202242488	0.32421392559553	-1.29676241700949
H	-3.88763332579112	-0.06613501381805	-1.25210970771400
C	-2.90174584358464	-1.95304601011501	0.76128269076284
H	-3.87579797038276	-1.75181886662120	0.33059737804788
C	-2.37266678616868	1.34569877030595	-2.01826414852063

H	-2.85356689480935	2.01114438173441	-2.71963040267273
C	-1.47575074986946	-3.15426453724054	2.26950159330426
H	-1.31218616209322	-3.90425884852448	3.03512378900037
C	-2.73749972328625	-2.93618617832767	1.72704830050529
H	-3.59095034405344	-3.51967978778961	2.05701807353732
C	-0.12647354090381	2.43370459248918	-2.34451640151197
H	0.42726032608865	2.98243887798365	-1.58111164027036
H	0.58588554178663	1.93683287336157	-3.00752073125134
H	-0.73894860673296	3.12847382897962	-2.92052292750197
C	1.92176947495870	2.50452777047884	2.16668841812608
H	2.87922695706901	1.98680794797747	2.25666029288920
H	1.94271215198975	3.17118542894357	1.30161307440458
H	1.67793194908442	3.03740619398894	3.09036995467936
C	-0.82578889810090	2.32945449420850	1.77032007228994
H	-0.70533098508196	2.97460820581724	0.89591635791075
H	-1.70629385350672	1.69063853245289	1.66894755942305
H	-0.89499042235550	2.91821620330208	2.68951902160425
N	2.52812874343200	-1.36893162884116	1.07421020032437
C	2.98111951824811	-1.23490474372401	2.33568978725067
C	3.13400062271232	-2.25671436843732	0.23926972434243
C	4.06856715734704	-1.94736299347849	2.81163346470583
H	2.42993176637500	-0.55360450596622	2.97773972225103
C	4.23530216822705	-2.99496977408063	0.66622776237739
C	4.71328975578454	-2.83468940057868	1.95840560251017
H	4.39828099201785	-1.80055473512358	3.83449199893813
H	4.72399342645681	-3.69358034783963	-0.00164193067841
H	5.57419268157771	-3.40337732498651	2.29583565788176
C	2.54601561941449	-2.38954781147496	-1.09907878371667
C	3.02100578499832	-3.27776051744348	-2.06264201598096
N	1.47491731958114	-1.59717343602707	-1.35720046480700
C	2.39533648538756	-3.35456806995842	-3.29704537643887
H	3.87711936242317	-3.90834712080353	-1.85728336438046
C	0.87109756793956	-1.67578433496695	-2.55400990988340
C	1.29691062975083	-2.54159600534937	-3.54662738410631
H	2.76189590997007	-4.04055538499636	-4.05387901397247
H	0.02404628015424	-1.01728102746280	-2.71429030526914
H	0.77551073671740	-2.56799542279812	-4.49729429228185

**3a<sup>+</sup>: [Ru(CN)(bpy)(Cl)(O-DMSO)]<sup>+</sup>**

Ru	0.76823671075798	-0.33624879859714	-0.01073583931933
Cl	2.42801923642403	1.28384027766209	-0.67978845980666
N	-0.74044375043802	-1.56192432594954	0.65338100676470
N	-1.99946696101067	-0.19611529928216	-0.68124385593539
C	-0.77201329578201	0.36715944908893	-1.02691337185997
C	-1.99124057263494	-1.24678112960256	0.22787805125801
N	-1.10138671056522	1.26052931640432	-1.99874573655865
C	-0.61555731007179	-2.59202008005498	1.51658446093599
H	0.39683089680849	-2.81890711733344	1.83392360919595
C	-3.04210543349746	0.34635045215815	-1.42600405500418
H	-4.07218671675048	0.04447442363953	-1.32865232810826

C	-3.12771838256172	-1.92299253753137	0.64907534897618
H	-4.10789557251038	-1.63288158030552	0.28796441349417
C	-2.47240233129198	1.26118670479060	-2.24064414778598
H	-2.92273443301706	1.91007357458725	-2.97648623122777
C	-1.69872273235214	-3.31730532966133	1.97465722776460
H	-1.53891604032884	-4.13714014936908	2.66583786943012
C	-2.97745879066615	-2.97585267164539	1.53870516638810
H	-3.84727486511647	-3.52387819383777	1.88498257206100
C	-0.15771007302078	2.14121137073386	-2.68390123887885
H	0.81741987975245	1.65539728666823	-2.72839221907975
H	-0.53138350850845	2.34522327144020	-3.69044368501915
H	-0.04273085011926	3.08161285471730	-2.13583535884074
N	2.33998015150385	-1.26124984510865	1.04648317293047
C	2.69182039222036	-1.01424701390703	2.31715291405315
C	3.11113693614312	-2.08053380569816	0.28884160502970
C	3.82198995164668	-1.56786757983588	2.89411043497585
H	2.03286382991771	-0.34187324564813	2.86021302544065
C	4.26644217778971	-2.66288123158698	0.81140962765746
C	4.62601799992442	-2.40399587514191	2.12416216996761
H	4.06976503354243	-1.33964284656017	3.92514336614108
H	4.88665718352513	-3.30667017934052	0.19915536051097
H	5.52461110539110	-2.84668710643770	2.54137622268427
C	2.61400885258961	-2.29965503546869	-1.06918442056757
C	3.22810279165292	-3.14905336407149	-1.98807914318618
N	1.46466151095445	-1.62889824919858	-1.38934488486888
C	2.67678177088031	-3.33181171841175	-3.24403598601283
H	4.14057473575682	-3.66716151084691	-1.71798479380858
C	0.93033344299106	-1.82396013153891	-2.61412250059281
C	1.49988452818542	-2.65723942925660	-3.55649294274854
H	3.15265744210167	-3.98821108420446	-3.96464401394523
H	0.01899189266461	-1.27544339401635	-2.82458085666386
H	1.02397593798784	-2.76789816995202	-4.52483785670237
O	0.29785329866418	0.90341423685141	1.67694510182790
S	0.31379425101879	2.45806935572744	1.44500356554224
C	1.82162953545945	3.04790763160635	2.28388092218678
C	-0.89408433598463	3.01611508618161	2.69112982208341
H	2.66307478814678	2.68391000042504	1.69074120705766
H	1.80477996928167	4.14223902887149	2.29537951709287
H	1.83960083148447	2.64488115850991	3.30034384010037
H	-0.86275942865576	4.10812860108202	2.75164825307050
H	-1.88027650502174	2.68913376901668	2.35388400172379
H	-0.65082846526163	2.56177017923879	3.65530007017595

**3a<sup>12+</sup>: [Ru(CN)(bpy)(Cl)(O-DMSO)]<sup>2+</sup>**

Ru	0.81109492455066	-0.16920464947891	-0.15749942846765
Cl	2.66620081605977	1.11011523122281	-0.70606740693007
N	-0.94942647617477	-1.23883661893595	0.23833552923716
N	-1.84617299495715	0.38491892306979	-1.11169885536782
C	-0.54784670157055	0.84510010170505	-1.24863663267462
C	-2.07710343957050	-0.73070619583599	-0.30839097345109

N	-0.65505791473024	1.88251464678905	-2.10613115763853
C	-1.04568423838950	-2.32791463803480	1.02657797568069
H	-0.11537164797718	-2.69987107845630	1.44321814081512
C	-2.73373428523908	1.13649147376650	-1.87577448246228
H	-3.79441841813443	0.95035120739144	-1.92656506852804
C	-3.32950854329124	-1.28564247404588	-0.08901610679569
H	-4.21719951745270	-0.85817237659243	-0.54074535304416
C	-1.97994909752717	2.07202841061990	-2.49258753090103
H	-2.26860770003859	2.85329163544900	-3.17972268248541
C	-2.25723190743058	-2.93551957216652	1.29324835025915
H	-2.29228594169124	-3.80992398478510	1.93316216734901
C	-3.41405821341793	-2.40529948194075	0.72552803553082
H	-4.37991885398947	-2.86307362343901	0.91469499620723
C	0.44930553907915	2.71715282904387	-2.59383011181283
H	1.24337421438034	2.08815933957187	-2.99845676420049
H	0.06412690371754	3.37328976652175	-3.37558167692669
H	0.85811098346930	3.31717703571459	-1.77802929246447
N	2.11445807402845	-1.38374536642629	0.99336657581392
C	2.43918841353512	-1.18354467543104	2.27820916794091
C	2.71818987507698	-2.37730464360703	0.29460499244307
C	3.37516414812366	-1.96910847541092	2.93196949902928
H	1.92484164194069	-0.36545570318749	2.77407490042543
C	3.66962748765938	-3.19886197752424	0.89663992615631
C	4.00133744648605	-2.99160713357638	2.22749765779467
H	3.61060362532768	-1.77504510101321	3.97281476112880
H	4.15536570491721	-3.98982098646697	0.33784059593066
H	4.74404512986619	-3.62031173013362	2.70808296726932
C	2.28901996550129	-2.50092389485541	-1.10105568599655
C	2.77260860709765	-3.46750267470896	-1.97972384991308
N	1.35472273403359	-1.59932621395777	-1.51877039720450
C	2.30577597161064	-3.51245204365492	-3.28389561908538
H	3.51622770635422	-4.18281471447238	-1.64973676091058
C	0.89959821356800	-1.64997062057117	-2.78514232410794
C	1.35012667030028	-2.58867414221025	-3.69397123154303
H	2.68429552724212	-4.26025110727177	-3.97339178237056
H	0.16243857971872	-0.90332806038231	-3.05970567868190
H	0.95916651749784	-2.58777894832026	-4.70549945110713
O	0.38933907685570	1.01344723586519	1.52521646507253
S	0.31767526832695	2.59194915551069	1.39293556948686
C	-0.92108498125879	3.02809579221304	2.64638481258876
C	1.81208667516653	3.17026046469966	2.25086517360469
H	-0.92224671157606	4.11660908904218	2.76165473258538
H	-0.66701865142886	2.53397035288581	3.58797410385077
H	-1.89363825256168	2.69193066716327	2.27995680277393
H	1.77120486551393	4.26342088804859	2.29878414543248
H	1.84252365324479	2.73469321987996	3.25317474194074
H	2.66681952815729	2.85222544072005	1.64951351872384